Physics-based Reconstruction of Sedimentary Rocks

Guodong Jin, UC Berkeley; Tad W. Patzek, SPE, UC Berkeley / Lawrence Berkeley National Laboratory; and Dmitry B. Silin, SPE, Lawrence Berkeley National Laboratory

Abstract

We develop a depositional model that reconstructs numerically the geometrical structure and mechanical properties of natural sedimentary rocks in two and three dimensions. Our emphasis is on unconsolidated sands and sandstones. Our model has the following distinctive features: (1) it accounts for the dynamic geologic processes of grain sedimentation and compaction, and the diagenetic rock transformations; and (2) it reproduces the mechanical rock properties. The main input parameters are the grain size distribution, the final rock porosity, the type and amount of cement and clay minerals, the coefficient of friction, the bond strength parameters, and the grain stiffness moduli. The initial grain shapes are circular in 2D and spherical in 3D. Our depositional model can also be used to study the initiation, growth, and coalescence of micro-cracks in the rock. The proposed approach makes it possible to model the accumulation of rock damage and fracture propagation. The development of micro-cracks in, for example, a 2D marble rock model is studied under increasing vertical stress. Both the box fractal dimension of the micro-crack distribution and its variation with the applied stress are estimated.

Introduction

Reconstruction of the void space of three-dimensional permeable rocks is of great interest in petroleum engineering. In the past decades, several approaches have been proposed to reconstruct the microstructure of natural porous media. An effective reconstruction procedure enables one to generate realistic rock images at will, and then modify these images to model the desired macroscopic properties (transport, electric, mechanical, etc.) of the rock.

Our goal is to obtain a reconstruction that resembles as closely as possible a given sedimentary rock with respect to its geometric and transport properties, and also its mechanical properties.

A promising approach to obtaining the microstructure of a rock is to simulate the relevant fundamental physical processes of rock formation, such as sedimentation, compaction, and diagenesis. Rock reconstruction completely specifies geometry of both the void space and the solid phase. Roberts and Schwartz introduced a grain consolidation model which simulates the diagenetic processes of cementation and compaction by increasing grain size uniformly. Bryant et al. developed a geologic model, which simulates the results of rock-forming processes using a completely defined packing of equal spheres constructed by Finney. Bakke et al. proposed a similar process-based reconstruction procedure to build the analogs of actual sandstones by stochastically modeling the results of the major processes of sandstone formation.

In natural rocks, the geometry of the solid skeleton and the structure of the void space are controlled by dynamic formation processes, which should be accounted for by a successful reconstruction of rock microstructure. Jia and Williams showed that when grains were allowed to rotate and/or rebound during sedimentation, a completely different structure of grain packing would result. In contrast, most process-based approaches mentioned above simulate the “final result” of rock-forming processes and ignore the dynamics of grain sedimentation. Finney’s
equal sphere pack was built to obtain a single random close packing of spheres, and ought not be used to generate different sedimentary rocks. Bakke et al.’s approach selects a “stable” position for the currently deposited grain at a local or global minimum of potential energy, and assumes that no lateral motion of other grains will result. Based on the initial grain packing, compaction is simulated by either shifting the coordinates of each grain in vertical direction by a distance that is proportional to its original position, or by just increasing the grain radii. These simplified models of compaction ignore the dynamic rearrangements of grain positions, and may produce a completely different microstructure of the simulated rock. In addition, in the simulations of rock cementation, the effect of grain size on the rate of cement overgrowth was mostly ignored.

Rock sedimentation and compaction are governed by gravity, contact forces, frictional forces from neighboring grains and surrounding fluids, and so on. The final sediment configuration depends on the forces and the force moments acting upon it. Few attempts have been made to account for the grain interaction forces and their moments during sedimentation and compaction. Wen and Chakrabarti\(^\text{20}\) accounted for the interparticle forces and translational motion, but not for the moments, damping forces, and rotational motion.

This paper describes how we reconstruct the two- and three-dimensional microstructures of simple sedimentary rocks: unconsolidated sands and sandstones. We simulate the dynamic processes of grain sedimentation and compaction with the distinct element method (DEM), proposed by Cundall and Strack.\(^\text{21}\) and model the results of diagenesis. The rock grain size affects the rate of cement overgrowth. The initial grain shapes are assumed to be circular in 2D and spherical in 3D.

DEM has been derived from molecular dynamics and simulates the dynamic interactions of discrete grains according to the fundamental laws of Newtonian physics. DEM explicitly takes into account the geometrical factors, and the forces and moments.\(^\text{21–23}\) It has been widely used to study mechanical behavior of granular materials, such as soils and powders, but has rarely been applied to reconstruct the microstructure of a sedimentary rock.

As a further test of our depositional model, a sample of the Tennessee marble rock\(^\text{24}\) has been reconstructed, and its mechanical behavior reproduced. The micro-crack development has been observed and its distribution analyzed using the box-counting method.\(^\text{25–28}\) Also, the effect of confining pressure and characteristic grain size has been quantified.

### Mechanisms of Grain Interactions

The bulk behavior of a grain system depends on the interactions of individual grains. Hence, grain-scale analysis should improve reconstruction of a porous medium.

The basic equations for a single grain in the multi-grain system are Newton’s equations of motion:

\[
F_i = m \ddot{u}_i \quad (1)
\]

\[
M_i = I \ddot{\theta}_i \quad (2)
\]

where \(u_i\) and \(\theta_i\) are the translational and rotational displacements of the grain in the \(i\) direction, \(i = x, y, z\); \(m\) is the mass of the grain; \(I\) is the moment of inertia of the grain; \(F_i\) and \(M_i\) are the resultant forces and moments acting on the grain.

The net force on a grain is a vector sum of the following forces: (i) **body forces**, \(F_{b,i}\), due to gravity and external forces acting on the grain; (ii) **contact forces**, \(F_{c,i}\), at the contact between the grains and between the grain and the boundaries; and (iii) **damping forces**

Two types of damping schemes are used in the simulation: velocity-proportional and stiffness-proportional. Velocity-proportional damping \((F_{dm,i})\) simulates energy dissipation by rock grains moving in the viscous fluids, and is assumed proportional to the grain velocity, \(\dot{u}_i\). Stiffness-proportional damping \((F_{sk,i})\) models energy dissipation during collisions of a grain with other grains or boundaries, and is assumed proportional to the velocity differences between the grains, \(\dot{u}_{c,i}\). These two damping forces can be expressed as

\[
F_{dm,i} = \alpha m \dot{u}_i \quad (3)
\]

\[
F_{sk,i} = \beta k \dot{u}_{c,i} \quad (4)
\]

where \(\alpha\) and \(\beta\) are the damping coefficients, and \(k\) is the contact stiffness.

When two grains come into contact under an external force, there will be deformation in the contact region, and the contact force will develop (Fig. 1a). The contact is simulated as a dash-pot, spring and slider system (Fig. 1b). In Fig. 1, \(x_{\text{A}}^{[A]}\) and \(x_{\text{B}}^{[B]}\) are the position vectors of grain A and B; \(x_{\text{C}}^{[C]}\) is the location of the contact point of these two grains; \(n_{\text{A}}\) is the unit normal vector defined from grain A to grain B; \(\mathbf{U}^n\) is the magnitude of deformation, which is assumed to be small compared with the grain size and linearly related to the contact force, unless slip or separation occurs between the grains; \(K^n\) and \(k^t\) are the normal and tangential contact stiffness; \(\mu\) is the friction coefficient.

![Schematic diagram of grain-grain contact and its relative contact model in the simulation.](image)
friction coefficient; and \( F_c \) is the contact force, which can be resolved into a normal and tangential component, \( F_n^c \) and \( F_t^c \) respectively,

\[
F_c = F_n^c + F_t^c
\]

The normal contact force, \( F_n^c \), is calculated by

\[
F_n^c = K_R U_n n_i
\]

The tangential contact force, \( F_t^c \), depends on the history of relative displacement, which is not entirely determined by the current grain locations. The relationship between the incremental tangential component of the contact force and the relative displacement is given by

\[
\Delta F_t^c = k^t \Delta U^t
\]

where \( \Delta U^t \) is the change of tangential component of the contact displacement of two grains.

For slip between two grains, the Mohr-Coulomb condition is used. Slip occurs between grains \( A \) and \( B \) when the normal and tangential components of the contact force satisfy the inequality

\[
|F_t^c| > c + \mu F_n^c
\]

where \( c \) is the cohesion coefficient. If slip occurs, the tangential contact force is changed to

\[
F_t^c := \begin{cases} \frac{F_t^c}{|F_t^c|} (c + \mu F_n^c) & \text{if slip occurs} \\ F_t^c & \text{if no slip} \end{cases}
\]

Finally, the equations of motion can be written as:

\[
\begin{align*}
\ddot{m} u_i + c m \dot{u}_i &= (F_{c,i} + F_{d,k,i}) + F_{b,i} \\
\ddot{I} \dot{\theta}_i + \alpha \ddot{\theta}_i &= (M_{c,i} + M_{d,k,i}) + M_{b,i}
\end{align*}
\]

where \( M_{c,i} \) and \( M_{d,k,i} \) are the moments of the contact forces and the contact damping forces; and \( M_{b,i} \) is the externally applied moment.

The dimensionless forms of Eqs. (10) and (11) are based on the following set of dimensionless variables:

\[
\begin{align*}
\bar{u} &= \frac{u}{R^*}, \quad \bar{\theta} = \theta, \quad \bar{k}^t = \frac{k^t}{K^*}, \quad \bar{F} = \frac{F}{F^*}, \quad \bar{M} = \frac{M}{M^*} \\
\bar{I} &= \frac{I}{I^*}, \quad \bar{\alpha} = \alpha \cdot T^*, \quad \bar{\beta} = \beta \cdot T^*, \quad \bar{\rho} = \frac{\rho}{\rho^*}
\end{align*}
\]

where \( R^*, K^* \), and \( \rho^* \) are the characteristic radius, stiffness and density of the largest grain in the packing; \( m^* = \rho^* R^3 \); \( T^* = \sqrt{m^*/K^*} \); \( I^* = m^* R^2 \); \( F^* = m^* g^* \); \( M^* = F^* R^* \) and \( g^* = g \). Eqs. (10) and (11) are now transformed to the following dimensionless form:

\[
\begin{align*}
\bar{m} \ddot{u}_i + c \bar{m} \dot{u}_i &= (\bar{F}_{c,i} + \bar{F}_{d,k,i}) + \bar{F}_{b,i} \\
\bar{I} \ddot{\theta}_i + \bar{\alpha} \ddot{\theta}_i &= (\bar{M}_{c,i} + \bar{M}_{d,k,i}) + \bar{M}_{b,i}
\end{align*}
\]

where \( C \) is the dimensionless parameter,

\[
C = \frac{T^* g^*}{R^*} = \frac{R^2 \rho^* g^*}{K^*}
\]

Numerical Time-Integration Schemes. The equations of motion (13) and (14) are solved numerically using a finite difference technique\(^{21,22} \) with a constant time step \( \Delta t \). The time step is chosen to be so small that no disturbance can propagate from any grain farther than its immediate neighbors. Therefore, it is assumed that grain velocities and accelerations are constant within each time step. The forces acting on any grain are then determined exclusively by its interactions with the grains with which this grain is in contact. The translational and rotational accelerations, and the velocities at time \( t \) are expressed in terms of the velocity values at mid-intervals. The accelerations are calculated as

\[
\begin{align*}
\dot{\bar{u}}_i^{(f)} &\approx \frac{1}{\Delta t} \left( \bar{u}_i^{(f+\Delta t/2)} - \bar{u}_i^{(f-\Delta t/2)} \right) \\
\dot{\bar{\theta}}_i^{(f)} &\approx \frac{1}{\Delta t} \left( \bar{\theta}_i^{(f+\Delta t/2)} - \bar{\theta}_i^{(f-\Delta t/2)} \right)
\end{align*}
\]

The velocities are calculated as

\[
\begin{align*}
\bar{u}_i^{(f+\Delta t/2)} &= \frac{1}{2} \left( \bar{u}_i^{(f+\Delta t/2)} + \bar{u}_i^{(f-\Delta t/2)} \right) \\
\bar{\theta}_i^{(f+\Delta t/2)} &= \frac{1}{2} \left( \bar{\theta}_i^{(f+\Delta t/2)} + \bar{\theta}_i^{(f-\Delta t/2)} \right)
\end{align*}
\]

Substituting these equations into the equations of motion (13) and (14), one obtains

\[
\begin{align*}
\bar{u}_i^{(f+\Delta t/2)} &= \left( A \bar{u}_i^{(f-\Delta t/2)} + \left[ (\bar{F}_{c,i} + \bar{F}_{d,k,i}) + \bar{C} \bar{F}_{b,i} \right] \bar{I} \Delta \bar{t} \right) B \\
\bar{\theta}_i^{(f+\Delta t/2)} &= \left( A \bar{\theta}_i^{(f-\Delta t/2)} + \left[ (\bar{M}_{c,i} + \bar{M}_{d,k,i}) + \bar{C} \bar{M}_{b,i} \right] \bar{I} \Delta \bar{t} \right) B
\end{align*}
\]

where

\[
\begin{align*}
A &= 1 - \alpha \Delta \bar{t}/2 \\
B &= \frac{1}{1 + \alpha \Delta \bar{t}/2}
\end{align*}
\]

Finally, the velocities calculated from Eqs. (20) and (21) are used to update the position and direction of the grain center:

\[
\begin{align*}
\bar{u}_i^{(f+\Delta \bar{t})} &= \bar{u}_i^{(f)} + \bar{u}_i^{(f+\Delta t/2)} \Delta \bar{t} \\
\bar{\theta}_i^{(f+\Delta \bar{t})} &= \bar{\theta}_i^{(f)} + \bar{\theta}_i^{(f+\Delta t/2)} \Delta \bar{t}
\end{align*}
\]

In this manner, the position of each grain and the forces acting on it can be explicitly tracked during grain sedimentation and compaction.

Simulation of Geological Processes

Sedimentary rocks are formed by a series of complex processes: source rock fragmentation, grain transport and erosion, sedimentation, and diagenesis. When energy of
a transporting medium becomes too low to continue the transport process, sediments begin to deposit. Once deposited, the sediments are compacted. Later, water flows through the deposited sedimentary bed dissolving, nucleating and growing solid materials by the processes called diagenesis. The diagenetic alteration cements the sediments into a solid rock.

Sedimentary rocks are reconstructed in three main steps: sedimentation, compaction and diagenesis, and their mechanical properties are matched. First, an initial grain packing is obtained by simulating the dynamic process of grain sedimentation. Some basic grain properties are needed for this step: the grain size distribution, the grain material density, the inter-particle friction coefficient, and the grain material stiffness coefficients. Second, the initial grain packing is compacted. Third, after compaction is completed, the end-result of diagenetic rock transformations is modeled and, e.g., cement bonds are introduced. Finally, suitability of the reconstructed rock to model mechanical properties of the real one is tested, and the mechanical-property input parameters are adjusted.

The first three steps of rock reconstruction are presented in this section, and the fourth is described in the section on rock damage.

**Sedimentation** Grain packing during sedimentation strongly affects the geometrical, transport, and mechanical properties of the resultant rock. The final grain packing is largely dependent on the grain size, shape, sorting and sedimentation environment. For example, poorly sorted grains have closer packing and lower porosity across a wide range of grain sizes, as the fine grains tend to fill the void space between the large grains.

The sedimentation process is simulated using a “generate-settle” algorithm. First, a predetermined number of grains is generated according to a given probability distribution function. Then, these grains are dropped into a given spatial domain either simultaneously or one-by-one, and either from one point or from randomly chosen positions. Alternatively, the generated grains are randomly placed within the domain according to some probability distribution function with overlaps or not. Thereafter, the grains settle under the action of gravity and other external forces, and reach a final equilibrium state. The final position of each grain depends on the forces and moments acting upon it.

Our DEM model simulates the dynamic process of grain sedimentation in which the grains are allowed to translate, rotate and rebound. **Fig. 2** shows a 2D 4 cm × 4 cm random grain packing which has already reached gravity equilibrium. Although any grain size distribution can be used, in this paper the grain sizes follow a truncated log-normal and uniform distributions.

The lognormal distribution is bounded by $R_{\text{max}} = 1.98 \text{ mm}$ and $R_{\text{min}} = 1.0 \text{ mm}$, and its mean and standard deviation are equal to 0.42 mm and 0.25 mm, respectively. The initial pixel-based porosity (the ratio of the number of pixels in the void space and the total number of pixels) is 15.01% (including the boundary effect). The pixel resolution is 0.1 mm.

**Fig. 3** displays a 3D 4 cm × 4 cm × 6.58 cm random grain packing after gravity-driven sedimentation. Here the grain sizes follow a uniform distribution bounded by $R_{\text{min}} = 1.8 \text{ mm}$ and $R_{\text{max}} = 2.7 \text{ mm}$. The initial voxel-based porosity (the ratio of the number of voxels in the void space to the total number of voxels) is 47.5% (including the boundary effect), while the porosity of a 1 cm × 1 cm × 1 cm sub-sample in the middle part of the grain pack is only 42.4%. The voxel resolution is 0.1 mm.

**Compaction** Compaction reduces rock bulk volume in response to the applied stress. Compaction forces grains closer to each other, and reduces the rock porosity. In quartz sandstones, compaction at shallow depths is mainly
caused by mechanical processes, such as grain rearrangement and grain fracturing. At greater depths, pressure dissolution is the main process causing compaction.

The compaction process is modeled by applying an overburden pressure and moving a wall at the top of a grain pack downwards by a certain distance. In this way, one simulates the effect of the overburden layers that apply stress on the reservoir. During compaction, a grain can undergo translational and rotational motion, depending on the forces and moments from its interactions with neighboring grains, confining boundaries, and surrounding fluids. Compaction modeling causes grains to interpenetrate, similarly to pressure dissolution of grain contacts in natural rocks. At present, we assume that the rock grains are very stiff, i.e., their interpenetration is very small, and the grain shapes do not change during compaction.

The grain interactions and rearrangement have a big influence on the final outcome of compaction. Fig. 4 shows the result of a 20% bulk volume reduction in uniaxial compaction of the 2D grain packing in Fig. 2. The positions of two grains, 1 and 2, are tracked during compaction. The origin of the coordinate system is in the lower-left corner, and the y-axis is oriented upwards. The initial positions of grain 1 and 2 are \((x_1, y_1) = (3.149, 3.328) \text{ cm}\) and \((x_2, y_2) = (0.639, 2.339) \text{ cm}\) (Fig. 2), and the final positions are \((x_1, y_1) = (3.231, 2.630) \text{ cm}\) and \((x_2, y_2) = (0.613, 1.925) \text{ cm}\) (Fig. 4). Therefore, even in a 2D packing, grains move in both vertical and horizontal directions.

If we assume that the volume of grain interpenetration during compaction has dissolved under pressure, the final pixel-based porosity is 4.23% after the compaction, compared with the initial 15.01%. As a comparison, two other approaches were also simulated: (i) the grains were allowed to move only in the y-direction, and (ii) the y-coordinate of each grain was shifted downwards by an amount proportional to its original position. These two approaches resulted in the final porosities of 5.36% and 5.80%, respectively. Fig. 5 depicts the result of compaction of the 3D grain packing in Fig. 3 after a 12.8% reduction of bulk volume in uniaxial compaction. The voxel-based porosity is 40.2%. Starting from the same initial packing and following the approach in Refs. 4–6 gives the porosity value of 45.6%. Both final porosities should be compared with the initial porosity of 47.5%, including the boundary effect. The porosity of a 1 cm \(\times\) 1 cm \(\times\) 1 cm sub-sample in the middle part of the grain pack is only 36.9%.

As expected, grain rearrangement in uniaxial compaction leads to a closer grain packing, and thus, to a lower porosity in both 2- and 3D grain packs.

**Diagenesis** Diagenesis turns an unconsolidated loose sediment into a rock. It involves all physical, chemical and biochemical processes that affect sediments between the time of deposition and metamorphism. Diagenesis mainly includes two types of processes: cementation and authigenesis.
Cementation is the process of mineral nucleation and precipitation which binds the rock grains. One of the most common types of silica cement is quartz overgrowth. Silica cement is precipitated on grains of the compacted rock and formed as syntaxial (or rim) overgrowth (Fig. 6). This type of cementation is simulated by using an improved algorithm, which is based on the grain-growth algorithm by Schwartz and Kimminau, but takes into account the effect of grain size on the rate of silica cement growth:

$$\Delta(\vec{r}) = \left( \frac{\bar{R}}{R_0} \right)^{\alpha} \min \left( \kappa l(\vec{r})^{\beta}, l(\vec{r}) \right)$$

(24)

where $\Delta(\vec{r}) = L(\vec{r}) - R_0$ is the increment of silica cement growth along the direction $\vec{r}$ measured from the grain center, $L(\vec{r})$ is the distance from the grain center to the pore-cement interface; $R_0$ is the original grain radius; $\bar{R}$ is the mean radius of grains in the sample; $l(\vec{r})$ is the distance between the original grain surface and the plane of the polyhedron (polygon in 2D) into which the grain is inscribed; $\alpha$ is the parameter which controls the effect of grain size on the rate of cement overgrowth; $\beta$ is the growth exponent which controls the direction of silica cement growth; and $\kappa$ controls the amount of porosity reduction.

The influence of $\alpha$ is shown in Fig. 8a-c. A positive value of $\alpha$ favors small-grain growth, with more cement deposited on the surfaces of the small grains (Fig. 8a). A negative value of $\alpha$ favors large-grain growth (Fig. 8c). If $\alpha = 0$, the grain size does not matter (Fig. 8b), and the same amount of cement is deposited on the surfaces of all grains. In general, the sign of $\alpha$ is arbitrary, negative, positive, or zero. From the physical point of view, a positive value of $\alpha$ seems more reasonable because the small grains have a larger specific surface area than the large grains. In this study, a positive value of $\alpha$ has been chosen to simulate silica cement growth.

The growth exponent, $\beta$, also affects the geometry of cement development (Fig. 8d-f). A positive value of $\beta$ favors pore-body growth, i.e., more cement is deposited toward the direction of a pore body or large distance, $l(\vec{r})$, (Fig. 8d). This type of cement growth tends to increase the ratio of pore surface-to-pore volume of the original pore space, and keeps the pore space interconnected even when porosity is very low. Negative value of $\beta$ favors pore-throat growth (Fig. 8f). In this situation, the silica cement preferentially deposits on the narrow grain contact regions, decreasing the pore surface-to-volume ratio. This growth tendency preserves a relatively high porosity when the pore space becomes disconnected. If $\beta = 0$, the growth is uniform, and the same amount of silica cement is deposited on grain surfaces in all directions (Fig. 8e).

Fig. 9 displays the result of cementation of the compacted 3D grain pack in Fig. 5. The parameters in Eq. (24) are $\alpha = 1.0$, $\beta = 1.0$, and $\kappa = 0.6$. The voxel-based porosity of a $1 \text{ cm} \times 1 \text{ cm} \times 1 \text{ cm}$ sub-sample from the middle part of grain packing is 17.8%. The voxel resolution is 0.1 mm. Compared with the porosity of 36.9% before the cementation, the sub-sample porosity is cut by half.
Fig. 8—Effects of the grain size parameter, $\alpha$, and the growth exponent, $\beta$, on the rate of quartz cement overgrowth in 2D. The original grain is grey, the quartz cement is black, and the void space is white.

(a) $\alpha = 2.0$
(b) $\alpha = 0.0$
(c) $\alpha = -2.0$
(d) $\beta = 1.0$
(e) $\beta = 0.0$
(f) $\beta = -1.0$

Fig. 11—The voxel-based pore space of a 1 cm $\times$ 1 cm $\times$ 1 cm sub-sample from the middle part of a grain pack at each stage of simulations, and the imaged pore space of a Fontainebleau sandstone. The cementations 1–3 are used to show the effect of growth exponent, $\beta$, on cement overgrowth. The value of $\kappa$ is adjusted to obtain the same porosity. The voxel resolution is 0.01 cm. (a) Sedimentation, $\phi = 42.4\%$, (b) Compaction, $\phi = 36.9\%$, (c) $\alpha = 1.0$, $\beta = 1.0$, $\kappa = 0.6$, $\phi = 17.8\%$, (d) $\alpha = 1.0$, $\beta = 0.0$, $\kappa = 0.032$, $\phi = 17.5\%$, (e) $\alpha = 1.0$, $\beta = -1.0$, $\kappa = 0.0022$, $\phi = 16.0\%$, (f) Fontainebleau sandstone, $\phi = 16.0\%$
changed at will to mimic the type of clays and the relevant depositional environment.

**Rock Damage Analysis**

An external stress can bring about grain fracturing and micro-crack development in a rock, and change the rock structure. It is useful to understand the interplay between the rock microstructure and the macroscopic rock properties such as porosity, permeability and rock strength. It is well known that nucleation, growth, interactions, and coalescence of micro-cracks determine rock failure and alter the macroscopic mechanical properties of the rock.

To understand deformation and fracture behavior of a rock, it is useful to observe evolution of micro-cracks in the rock, and characterize patterns in the spatial distribution of these micro-cracks. Efforts have been made by many researchers to observe and analyze the micro-crack development in stressed rocks, e.g., Refs. just to name a few.

A reconstruction of the Tennessee marble rock is performed and its mechanical behavior is reproduced. The reconstructed rock is used to study the initiation, growth, and coalescence of micro-cracks in a compressional test. The pattern of micro-crack distribution is analyzed by the box-counting technique.

**Descriptions of Rock Sample and Test Condition.**

A 3.17 cm × 6.34 cm model of Tennessee marble rock is created from 4,860 grains (Fig. 13). The grain sizes are assumed to follow the uniform distribution bounded by $R_{min} = 0.25 mm$ and $R_{max} = 0.415 mm$. Uniform properties are assigned to the grains: the density, $\rho = 2,630 kg/m^3$, the coefficient of friction, $\mu = 0.33$, and the normal and tangential stiffness, $k_n = 1.0 \times 10^8 N/m$, and $k_t = 1.0 \times 10^8 N/m$, respectively. These property values were already used in the simulation of grain sedimentation and compaction.

Neighboring grains in the rock are connected by contact bonds that approximate the physical behavior of the cement filling the grain contacts and joining the grains. Each bond is assumed to be ideally fragile, i.e., to have a linear elastic response up to the threshold normal strength, $S_n$, or shear strength, $S_s$, at which it breaks. The threshold normal and shear strengths are assumed to be distributed randomly according to the normal distributions with the means of 155 MPa and 140 MPa, and the standard deviations of 35 MPa and 25 MPa, respectively. A bond is irreversibly broken once the stress acting on it is larger than its threshold strength. In this study, each bond breakage is assumed to result in a micro-crack, which could close but cannot be healed during the experiment, i.e., the micro-crack always exists after its inception. At present, the grains are assumed to be much stronger than the bonds. Thus, the individual grains are not breakable during the test.

The sample is loaded by applying the force that moves the top and bottom walls toward each other at a constant velocity of 0.2 m/s. Also the constant confining pressure,
Fig. 13—Sample geometry of the reconstructed Tennessee marble rock (4,860 grains, 9,562 bonds). The thin lines show the locations of bonds located between and joining the grains in contact.

Fig. 14—The stress-strain response of the reconstructed marble rock and the increase of the number of micro-cracks with axial strain in the test. The laboratory data are from Wawersik and Fairburst.24 The total number of micro-cracks should be multiplied by 10.

Results with $P_3 = 6.9$ MPa. The stress-strain response of the reconstructed rock is shown in Fig. 14. The numerical result is very similar to that obtained in the laboratory test. The macroscopic Young’s modulus and peak strength are approximately reproduced by the reconstructed rock. The variation of the total number of micro-cracks with axial strain is also shown in this figure. It can be seen that most micro-cracks form after the peak stress has been reached.

Fig. 15 shows evolution of the distribution of micro-cracks in the reconstructed marble rock by depicting the orientations and locations of the micro-cracks at strains of 0.15%, 0.20% (pre-peak), 0.274% (peak), and 0.364% (post-peak), respectively. At first, few micro-cracks randomly distributed over the sample area develop. When approximately 3.6% of the bonds are broken, micro-cracks start to interact and coalesce. Finally, numerous micro-cracks link together to develop shear localization, and the rock fails. Most of the micro-cracks form along linear bands after the peak stress is reached. The progressive development of micro-cracks and the final shear macro-fracture formation are consistent with the laboratory observations that generally show failure of samples along inclined shear fractures.

The distribution of micro-cracks is analyzed by using the box-counting or box dimension technique.25 Fig. 16 and Fig. 17 show the number of boxes, $N$, needed to cover the micro-cracks vs. the box size, $a$, when the rock is subjected to different stresses. The log of $1/a$ is used to

\[ P_3 = 6.9 \text{ MPa}. \]

The loading rate is slow enough to ensure that the sample remains in quasi-static equilibrium throughout the test and inertial effects can be neglected.

$P_3 = 6.9 \text{ MPa}$. The stress-strain response of the reconstructed rock is shown in Fig. 14. The numerical result is very similar to that obtained in the laboratory test. The macroscopic Young’s modulus and peak strength are approximately reproduced by the reconstructed rock. The variation of the total number of micro-cracks with axial strain is also shown in this figure. It can be seen that most micro-cracks form after the peak stress has been reached.

Fig. 15 shows evolution of the distribution of micro-cracks in the reconstructed marble rock by depicting the orientations and locations of the micro-cracks at strains of 0.15%, 0.20% (pre-peak), 0.274% (peak), and 0.364% (post-peak), respectively. At first, few micro-cracks randomly distributed over the sample area develop. When approximately 3.6% of the bonds are broken, micro-cracks start to interact and coalesce. Finally, numerous micro-cracks link together to develop shear localization, and the rock fails. Most of the micro-cracks form along linear bands after the peak stress is reached. The progressive development of micro-cracks and the final shear macro-fracture formation are consistent with the laboratory observations that generally show failure of samples along inclined shear fractures.

The distribution of micro-cracks is analyzed by using the box-counting or box dimension technique.25 Fig. 16 and Fig. 17 show the number of boxes, $N$, needed to cover the micro-cracks vs. the box size, $a$, when the rock is subjected to different stresses. The log of $1/a$ is used to
Fig. 15— The distribution of micro-cracks in the reconstructed marble rock during the uniaxial test at a strain of (a) 0.150% (pre-peak) (b) 0.200% (pre-peak), (c) 0.274% (peak), and (d) 0.364% (post-peak).

Fig. 17— The dependence of the number of boxes, $N$, needed to cover the micro-cracks on box size, $a$, in the post-peak stage of the test. (6) $\epsilon = 0.274\%$, $D = 0.85$, (7) $\epsilon = 0.291\%$, $D = 1.06$, (8) $\epsilon = 0.30\%$, $D = 1.05$, (9) $\epsilon = 0.316\%$, $D = 1.12$, (10) $\epsilon = 0.336\%$, $D = 1.15$, (11) $\epsilon = 0.364\%$, $D = 1.22$. The log of $1/a$ is used to obtain the fractal dimension, $D$.

Fig. 18 and Fig. 19 show the variation of the estimated fractal dimension $D$ with axial strain and deviatoric stress. It can be observed that the estimated fractal dimension of micro-cracks in the reconstructed marble rock always increases with the increasing axial strain. The fractal dimension also increases with the deviatoric stress until the peak stress is reached, and it continues to increase with the decreasing deviatoric stress beyond the peak stress. This behavior is consistent with Carpinteri and Yang’s observations of disordered materials. No critical value is found for the fractal dimension even when the reconstructed marble rock fails. The increasing fractal dimension during the test means that the rock becomes filled with cracks as the bond damage propagates.

The fractal dimension $D$ can be approximated as a function of the axial strain,

$$D = -4.94(100\epsilon)^2 + 7.20(100\epsilon) - 0.70$$

and as two functions of the normalized pre- and post-peak stress:

$$D = 7.37\bar{\sigma}^3 - 12.83\bar{\sigma}^2 + 7.54\bar{\sigma} - 1.21$$
$$D = -14.42\bar{\sigma}^3 + 32.55\bar{\sigma}^2 - 24.75\bar{\sigma} + 7.47$$

where $\epsilon$ is the axial strain, $\bar{\sigma}$ is the normalized stress, $\bar{\sigma} = \sigma/\sigma_0$, and $\sigma_0$ is the peak deviatoric stress.
Effects of Characteristic Grain Size and Confining Pressure. It is known that characteristic grain size and confining pressure influence the mechanical behavior and transport properties of rocks. In order to study the influence of grain size and confining pressure on the fractal dimension of the micro-crack distribution in the reconstructed rock, three other computer experiments were performed: the first two using the same marble rock as above, but under different confining pressures, $P_3 = 10 \text{ MPa}$ and $P_3 = 20 \text{ MPa}$; and the third one under the constant confining pressure, $P_3 = 6.9 \text{ MPa}$, but with the grain radii decreased by half and, thus, the total number of grains and contact bonds increased to 9,376 and 18,606, respectively, compare Figs. 4 and 13. All other rock properties have remained the same.

Since fracture formation is generally irreversible (at least over a short time period), the process is cumulative and can be described using the so-called state variables or damage parameter, which increase monotonically during the progressive bond failure. The formation of the shear macrofracture in the reconstructed rock results from the initiation, interactions, and coalescence of micro-cracks, i.e., broken bonds. Thus, the damage parameter may be defined as the ratio of the number of broken bonds, $n_f$, to the total number of bonds, $n$, in the rock sample:

$$DP = \frac{n_f}{n} \quad (28)$$

The variation of the damage parameter, or the fraction of broken bonds, with axial strain is shown in Fig. 20. It can be seen that the confining pressure has little effect on the variation of damage parameter for the same rock, and the effect of characteristic grain size can also be ignored although using different grain sizes means creating a differently scaled rock.

Fig. 21 shows the fractal dimension of the micro-crack distribution vs axial strain for different confining pressures and grain sizes. For the same rock, the confining pressure has negligible effect on the fractal dimension until the axial strain is about 0.25% at the peak stress. Grain size
has a certain effect on the fractal dimension of the micro-crack distribution. The fractal dimension decreases with the increasing grain size, in agreement with Babadagli and Develi’s observations.45

The effect of confining pressure and characteristic grain size can also be seen from the distribution patterns of micro-cracks at the final stage of rock failure. Fig. 22. The rock has nearly the same distribution pattern of micro-cracks under different confining pressures (Note that the rock fails at different axial strains.) The rocks with the different grain sizes show different failure patterns that result in different variations of the fractal dimension.

Conclusions

We have developed a general, process-based approach for reconstructing simple sedimentary rocks: unconsolidated sands and sandstones. The reconstruction procedure consists of three main steps, sedimentation, compaction and diagenesis, followed by reproduction of mechanical rock properties. The essence of our approach is to build analogs of real sedimentary rocks by simulating the dynamic processes of grain sedimentation and compaction, modeling the result of diagenesis process, and reproducing the mechanical behavior of the simulated rock.

The dynamic processes of grain sedimentation and compaction are simulated by solving the dimensionless form of Newton’s equations of motion for each grain in a grain pack. The grains in the pack may be subject to external forces, such as gravity, damping forces from the viscous fluid, and they may interact with each other through classical compressional and frictional contact forces. At present, the contact between grains is modeled as a dash-pot, spring and slider system, and the contact force is assumed to be linearly related to the magnitude of the deformation at the contact. More realistic interparticle relationships between the forces and displacements are under implementation using the Hertz-Mindlin theory.46,47

A meaningful reconstruction approach should preserve as many attributes of the real rock as possible. Thus, not only the geometrical and transport properties of the real rock, but also its mechanical properties should be reproduced. The key feature of our approach is that it requires to first match the mechanical behavior of the target sedimentary rock, then quantitatively compare the important morphological and transport properties of the reconstructed and real rock samples. Only when all these properties are nearly matched, does the reconstruction procedure finish.

Our approach enables one to study the process of progressive rock failure, and secondary porosity generation. For example, the reconstructed Tennessee marble rock shows many features of rock damage observed in laboratory tests, such as micro-crack initiation, interactions, coalescence, and shear macrofracture formation. Our results confirm that it is possible to reconstruct some sedimentary rocks so that their geometrical, transport, and mechanical properties are matched simultaneously.

Fractal geometry may be useful in explaining the progressive damage and rock failure during a rock deformation process. The self-organized distribution of the micro-cracks developed in the reconstructed rock displays fractal properties throughout uniaxial compression tests. The increasing fractal dimension during these tests shows that the reconstructed rock becomes more disordered with damage evolution.

This study is but a first step towards obtaining an industrial strength 3D depositional models and extracting meaningful rock transport properties from these models. The simulated results will be compared with laboratory measurements for a variety of sedimentary rocks. We believe that our approach is (1) physically sound, and (2) we can study the evolution of sedimentary rock microstructure (its porosity, permeability, and strength) during arbitrary rock deformations, thus enhancing general understanding of the deformation and fracture behavior of oil and gas reservoirs.

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References

Fig. 22—Distribution of micro-cracks in the rock when it fails at different confining pressures (a–c), and with different grain sizes under the fixed confining pressure, \( P_3 = 6.9 \text{ MPa} \) (d).


