DEM and SC estimations of elastic moduli of complex rock matrix using composites as analogs
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Summary
At low porosity, the elastic moduli of the rock mineral matrix often dominates those of the whole rock. A sedimentary rock matrix may be considered as a composite and may include mineral constituents with very different moduli and shapes. To describe the fabric of these rocks, an unmanageable number of parameters may be needed. Understanding the elastic behavior of synthetic composites, which are easier to model, enables us to quantify the effect of each parameter on the elastic moduli of the rock matrix independently. We test whether the differential effective-medium (DEM) and self-consistent (SC) models can accurately estimate the elastic moduli of a complex rock matrix and compare the results with the average of upper and lower Hashin-Shtrikman bounds (HS). The testing was conducted using data from the literature on composites, covering a wide range of inclusion concentrations, inclusion shapes, and elastic modulus contrasts. We find that when the microstructure is consistent with the DEM approximation, DEM is more accurate than both SC and the bound-average method for a variety of inclusion aspect ratios, concentrations, and modulus contrasts. If relatively little information is known about the rock microstructure, DEM can estimate the elastic properties of complex mixtures of minerals more accurately than heuristic estimates, such as the arithmetic average of the upper and lower elastic bounds.

Introduction
Composites can be fabricated with several constituent phases. The simplest are two-phase composites. Two-phase composites, including granular aggregates such as polycrystalline aggregates, can be classified in terms of the phase continuity and connectivity. Three main composite categories have been suggested (Ji and Xia, 2003; Gurland, 1979): a) composites with a stiff-phase-supported frame (SPSF), in which the stiff phase is continuous, while the compliant phase is discontinuous in the direction of the applied load; b) composites with a compliant phase-supported-frame (CPSF), in which the stiff phase is discontinuous while the compliant phase is continuous in the loading direction; and c) composites with a transitional frame (TF), in which both the stiff and the compliant phases are continuous (TFC) or discontinuous (TFD) in the loading direction. When all phases are discontinuous, there is no well-defined matrix phase, such as in completely random polycrystalline materials. In this study, to model the elastic moduli of materials, we consider effective-medium models, which are based on wave scattering theory. Specifically, we consider a self-consistent model (SC) known as the coherent potential approximation (CPA) (Berryman, 1980; 1995) and a differential effective-medium (DEM) approximation (Norris, 1985). We test the effective-medium models on a large data set of CPSF and SPSF composites in order to evaluate their predictions for a wide range of elastic moduli contrasts and inclusion shapes, with the goal of finding which model will most accurately determine the effective elastic moduli of sedimentary rocks with complex matrices. For testing the accuracy of the DEM and CPA models, compared with the Hashin-Shtrikman bounds (Hashin and Shtrikman, 1963), we used twenty-three two-phase composite experimental data sets from the literature. These composites cover a wide range of inclusion concentrations and elastic-modulus contrasts.

Comparison of theoretical and experimental data
Figures 2-5 show the measured elastic properties and theoretical predictions for the two-phase composite data sets. For the application of DEM described in this subsection, the aspect ratio of the inclusions was 1, and for CPA the aspect ratio was 1, for both host and the inclusions. In most of the composites, the experimental
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velocities fall inside the Hashin-Shtrikman bounds. At small inclusion concentrations, the lower Hashin-Shtrikman bound ($HS^-$) gives accurate results for the CPSF composites, and the upper Hashin-Shtrikman bound ($HS^+$) gives accurate results for the SPSF composites. At low concentrations, the DEM, CPA and DL predictions for CPSF composites with aspect ratios close to unity approach the lower Hashin-Shtrikman bound ($HS^-$). For SPSF composites the model predictions approach the upper Hashin-Shtrikman bound ($HS^+$). At high concentrations, the difference between the model predictions and $HS^-$ or $HS^+$ increases. For the entire range of inclusion concentrations, the predictions of DEM and CPA lie between the $HS$ bounds.

Figure 1: Tomographic slices of a 3D CT-scan image of tight gas sandstone. Upper: micro-CT resolution. The pore space is not discernable. The elements of varying density, from high (white) to low (dark gray) are apparent. Lower: nano-CT resolution. The micropores appear black and embedded into light-gray crystals. White crystals represent high-density and high-stiffness mineral. The dark-gray (lower-density) background is relatively soft. Courtesy Ingrain, Inc.

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Notice that as concentration increases, the prediction accuracy for all models deteriorates. The inclusions in most of the composites are spheroidal and have different ranges of particle sizes (highly polydispersed). When small particles are present, they usually tend to agglomerate in clusters, such as in the cobalt-tungsten-carbide (Co/WC) system, even for low concentration values (Sahimi, 2003). As particle size increases, the tendency for clustering is reduced. At high concentration, the inclusion phase becomes more continuous because the degree of connectivity between particles increases. As the inclusion volume fraction increases, more inclusions aggregate to form clusters. The volume fraction at which the first single cluster of inclusions spans the sample is called the percolation threshold volume. Depending on the contrast between the host and inclusion velocity, this single cluster may be the fastest (or slowest) way for a wave to propagate through the sample, for wavelengths that are smaller than the cluster size. At the percolation threshold, a transition occurs in the effective elastic properties of the material (Stauffer and Aharony, 1994; Gomez et al., 2000; Nur et al., 1998).

Effective-medium models apply only to statistically homogeneous media. A moderately heterogeneous material may be assumed to be statistically homogeneous. Thus there exists a representative elementary volume (REV), and any part of the statistically homogeneous system with a volume considerably larger than the REV has identical physical properties (Gueguen et al., 1997; Gueguen et al., 2006). Decreasing the oblate inclusion aspect ratio is equivalent to increasing the connectivity between inclusions, such as in rocks with large number of fractures, or clustering of inclusions in composite materials. Thus, the percolation threshold will be reached earlier in materials with low-aspect-ratio inclusions than in those with high-aspect-ratio inclusions. The change in continuity or connectivity of the inclusion phase occurs gradually. The rate of this change, as more inclusions are added to the material, depends on the size and shape spectra of the inclusions. CPA gives a percolation transition of 0.59 for spherical inclusions.
Accuracy of DEM and SC estimations

Figure 2. Top row: measured and calculated effective density of the materials. Middle and bottom row: comparison of ultrasonic experimental to calculated effective $V_p$ and $V_s$ velocities, respectively. The aspect ratio used in DEM and CPA was 1. These two composites are of the CPSF type. Left column: laboratory data from Bridge and Cheng (1987). Right column: data from Lees and Davidson (1977).

Conclusions

We find DEM provides consistently accurate predictions for all analyzed composites in a wide range of volumetric concentration.

At low concentrations (~0.10), if the rock’s microstructure is comparable with CPSF- or SPSF-materials, Hashin-Shtrikman bounds can be used as good predictors of elastic properties.

If a sedimentary rock’s microstructure is comparable with CPSF- or SPSF-materials and some information about the grain (inclusion) spectrum is known, it is better to use effective-medium models to estimate the elastic properties of the rock matrix at all inclusion concentrations, instead of averaging the upper and lower Hashin-Shtrikman bound. These results are intended to be used as a rigorous foundation for further effective-medium modeling of sedimentary rock.

Figure 3. Top row: measured and calculated effective density of the materials. Middle and bottom row: comparison of ultrasonic experimental to calculated effective $V_p$ and $V_s$ velocities, respectively. The aspect ratio used in DEM and CPA was 1. These two composites are of the CPSF type. Left column: laboratory data from Zhang et al. (1996). Right column: data from Piche and Hamel (1986).
Accuracy of DEM and SC estimations

Figure 4. Top row: measured and calculated effective density of the materials. Middle and bottom row: comparison of ultrasonic experimental to calculated effective $V_p$ and $V_s$ velocities, respectively. The aspect ratio used in DEM and CPA was 1. This composite is of the CPSF type. Laboratory data from Lees (1973).

Figure 5. Top row: measured and calculated effective density of the materials. Middle and bottom row: comparison of ultrasonic experimental to calculated effective $V_p$ and $V_s$ velocities, respectively. The aspect ratio used in DEM and CPA was 1. These two composites are of the CPSF type. Left column: laboratory data from Nguyen et al. (1996). Right column: data from Sugawara et al. (2005).

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REFERENCES


