Differential Effective Medium Modeling of Rock Elastic Moduli with Critical Porosity Constraints

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Abstract. Rocks generally have a percolation porosity or critical porosity at which they lose rigidity and fall apart. Percolation behavior is a purely geometrical property, independent of any physical properties, and is a powerful constraint on any valid velocity-porosity relation. We show how the conventional Differential Effective Medium (DEM) theory can be modified to incorporate percolation of wave velocities and elastic moduli in rocks. This is done by taking the material at the critical porosity as one of the constituents of a two-phase composite. Any desired percolation porosity can be specified as an input. In contrast, the conventional DEM model always predicts percolation at a porosity of either zero or one hundred percent. Most sedimentary rocks however have intermediate percolation porosities and are therefore not well represented by the conventional theory. The modified DEM model incorporates percolation behavior, and at the same time is always consistent with the Hashin-Shtrikman bounds. The predictions of the modified theory compare favorably with laboratory sandstone data.

Introduction

General relationships between seismic velocities and porosities in rocks are of great interest, not only from the theoretical point of view, but also for practical applications in seismic mapping and characterization of subsurface reservoirs. Various effective medium formulations that model the rock as a multiphase composite have been used to estimate theoretically the velocity-porosity relation in rocks (e.g. Wang and Nur, 1992 and references therein). Any model that accurately relates elastic wave velocities to porosity in rocks must incorporate two simple and almost universal observations: (1) Rocks generally have their highest elastic moduli and seismic velocities in the limit of zero porosity, approaching the moduli of the mineral constituents, and (2) there is almost always a finite *critical porosity* or percolation porosity, ϕ_c, at which the rock loses its rigidity and falls apart (O'Connell and Budiansky, 1974; Berryman, 1980; Nur, 1992). In addition, it is desirable that the model predictions always lie within known, rigorous bounds [such as the

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Hashin-Shtrikman (1963) bounds] on bulk and shear moduli. While virtually all theoretical models (and some empirical ones) have the correct mineral limit at zero porosity, only a few, including most notably the self-consistent (SC) models, also incorporate percolation behavior (Wu, 1966; O'Connell and Budiansky, 1974; Berryman, 1980). The conventional differential effective medium (DEM) formulations used for modeling composites do not have this percolation property (Norris, 1985; Zimmerman, 1991; Berge et al., 1993). Furthermore, only the DEM and one of the SC models based on the coherent potential approximation (Berryman, 1980) have been shown to be realizable for ellipsoidal inclusions (Milton, 1985; Norris, 1985; Avellaneda, 1987), and are therefore always consistent with the Hashin-Shtrikman bounds.

The largely successful self-consistent models are parametrized by the aspect ratio, α, (or aspect ratio spectrum) of the ellipsoidal inclusions. It is not easy to pre-specify the desired critical porosity as an input; one has to accept whatever value of ϕ_c happens to come out of the calculations with a given α. While almost any velocity-porosity trend can be obtained by simply varying the aspect ratio, in real rocks the appropriate aspect ratio spectrum is rarely easy to determine. Furthermore, the aspect ratio of an ellipsoid is not always a natural descriptor of the complicated pore microgeometry. Practically speaking, for irregular grain and pore shapes it is only through empirical curve fitting that the equivalent aspect ratio can be determined.

In contrast, the critical porosity is more readily observable from the general trend of the modulus-porosity data within restricted classes of rock samples (Nur, 1992). The percolation porosity is determined by the way the rock and pore space are formed and is a more natural descriptor of the pore space. We usually know more about the appropriate limiting value of ϕ_c than about the equivalent aspect ratio spectrum for a particular rock. Moreover, the percolation behavior of porous rocks is a purely geometrical phenomenon, independent of electrical or elastic properties of rocks. Therefore it is a powerful, model-independent input to any valid, physically reasonable velocity-porosity relation. Hence it is advantageous to have models that specifically incorporate this knowledge of ϕ_c, and at the same time are guaranteed never to violate bounds, including the Hashin-Shtrikman bounds.

In this paper we focus on how, by a simple redefinition of one of the end members, the DEM formulation can be modified to include any percolation porosity as a convenient input for modeling rock elastic properties. In addition, the estimates are assured always to be consistent with the Hashin-Shtrikman bounds, since DEM is a realizable model. Instead of the pure mineral and pore fluid, we take the pure mineral and a composite of mineral and fluid at the critical porosity as the new end members in the modified DEM formulation. As an example, we compare the theoretical predictions with laboratory data on sandstones (Han, 1986; Jizba, 1991), and show that the modified DEM results fit the observations reasonably well.

Critical Porosity

The critical (percolation) porosity marks a qualitative and quantitative transition in the state of the porous rock, with a distinct change in the physical properties (Chen, 1992). Laboratory and in situ data indicate such transitions in effective elastic moduli and wave velocities (Marion and Nur, 1989; Murphy et al., 1993; Nolen-Hoeksema, 1993), permeability and electrical conductivity (Bernabe et al., 1982; Walder and Nur, 1984), and strength (Kendall, 1984; Jizba, 1991). The percolation porosity for different physical properties need not be the same. We will be concerned only with the critical porosity, ϕ_c, for effective elastic moduli and wave velocities. Below ϕ_c, the mineral grains are load-bearing. Above ϕ_c, the pore fluid becomes load-bearing, and the material behaves mechanically like a suspension. A dry rock falls apart above ϕ_c. At the percolation porosity, the material is a loose packing of grains barely touching each other. We will define this to be the critical phase [sometimes also termed the critical concentration phase (Chen, 1992)]. Here the term "phase" has no chemical connotations.

The critical porosity is a geometric property that is determined by the process of formation of the rock and the pore microgeometry (Nur, 1992; Guégen and Palciauskas, 1994). Each class of rocks, depending on its genesis and evolution, has a particular critical porosity. Clastics—ranging from low porosity sandstones to high porosity unconsolidated sands—have a critical porosity representative of the originally deposited sediments and sand grains before diagenesis, typically $\phi_c \sim 0.36 - 0.40$. This is close to the porosity for a random close packing of spheres (0.36). Chalks have a critical porosity of $\phi_c \sim 0.6 - 0.7$ which is the sum of the $\sim 0.36 - 0.40$ intergranular porosity of clastics, plus an additional $\sim 0.2 - 0.3$ microporosity within the skeletal grains. In vesicular volcanic rocks, the nearly spherical pores formed by outgassing result in a glass foam that can stay intact to a $\phi_c \sim 0.9$ or more. Crystalline rocks such as granites and quartzites, where the porosity is primarily in the form of microcracks, can have a critical porosity of only $0.02 - 0.05$. It takes only a few percent, by volume, of cracks before a rock will fall apart.

The elastic moduli of the critical phase at ϕ_c depend on factors such as the sorting of the grains and the confining pressure. For very low confining pressures, the elastic moduli at the percolation point are equal to the Reuss average (harmonic average) of the moduli of the constituents. This is because the material is a suspension and is under iso-stress conditions.

The simplest curve that passes through the mineral modulus at $\phi = 0$ and the critical phase modulus at $\phi = \phi_c$ is a straight line. It does a surprisingly good job of predicting seismic velocities in clean sandstones at high confining pressures (Nur et al., 1991). This *modified Voigt* line amounts to redefining the end members and the weighting factors for the Voigt average (arithmetic average) (Nur et al., 1991; Chen, 1992). Instead of pure mineral and pure fluid, the pure mineral and the critical phase at ϕ_c are taken as the two constituents. Nevertheless it is a heuristic model, and for sufficiently large values of ϕ_c, the modified Voigt equation can give estimates that sometimes violate the Hashin-Shtrikman bounds. Its appeal is its simplicity and the good fit to high pressure data.

The idea of taking the critical phase as one of the end members has been used to modify various other existing analytical and empirical relations such as the Hashin-Shtrikman upper bound, Wyllie's relation and Mori-Tanaka's inclusion model (Chen, 1992). The modified Hashin-Shtrikman formula, of course, satisfies the bounds, and also shows a good fit to high pressure data. We use the same concept and modify the DEM formulation to model rocks with percolation behavior. The modification is implemented by 1) replacing the inclusion phase by the critical phase and 2) renormalizing the porosity to ϕ/ϕ_c. Sheng (1991) introduced a somewhat similar 3-component DEM method for modeling electrical and elastic properties of rocks. For his starting material he uses a mixture of fluid and cement, with the fluid fraction restricted to lie between 0.4 and 0.6. Furthermore, his model is restricted to very specific grain shapes, motivated by a desire to attain agreement with Archie's law for electrical conductivity. This philosophy and its implementation is very different from the one presented here, leading to restrictions on the range and ease of applicability that our theory does not share. Finally, it should be remembered that using the critical phase as one of the constituents does not model in all detail the complex microstructure and geometry of the pores, cracks, and grains, pore-to-pore interaction and connectivity, and the effects of overgrowths, cementation, and diagenesis. It is just a convenient way to incorporate critical porosity as an input to existing models.

DEM with Critical Porosity Inputs

The differential effective medium theory models two-phase composites by incrementally adding inclusions of one phase (phase 2, say) to the matrix phase. The matrix begins as phase 1 (when concentration of phase 2 is zero) and is changed at each step as a new increment of phase 2 material is added. The process is continued until the desired proportion of the constituents is reached. The actual calculations of the effective bulk and shear moduli are done by solving an initial value problem for a coupled system of ordinary differential equations. For thorough reviews of the DEM theory see Cleary et al. (1980), Norris (1985), and Zimmerman (1991). The DEM formulation does not treat each constituent symmetrically. There is a preferred matrix or host material, and the effective moduli depend on the construction path taken to reach the final composite (Norris, 1985). Starting with material 1 as the host and incrementally adding inclusions of material 2 will not, in general, lead to the same effective properties as starting with phase 2 as the host. For multiple inclusion shapes or multiple constituents, the moduli of the final composite depend not only on the final volume fractions of the constituents but also on the order in which the incremental additions are done. The process of incrementally adding inclusions to the matrix is really a thought experiment and should not be taken to provide an accurate description of the true evolution of rock porosity in nature.

The coupled differential equations for the effective bulk and shear moduli, K^* and μ^*, respectively, are (Berryman, 1992; Berryman and Berge, 1993):

$$(1-y)\frac{d}{dy}[K^*(y)] = (K_2 - K^*)P^{(*2)}(y) \tag{1}$$

$$(1-y)\frac{d}{dy}[\mu^*(y)] = (\mu_2 - \mu^*)Q^{(*2)}(y) \tag{2}$$

with initial conditions $K^*(0) = K_1$ and $\mu^*(0) = \mu_1$, where K_1, μ_1 are the bulk and shear moduli of the pure initial host material (phase 1), K_2, μ_2 are the moduli of the other end member (the incrementally added inclusion phase, phase 2), and y is the concentration of phase 2. For fluid inclusions and voids, $y = \phi$, the porosity. The factors $P^{(*2)}$ and $Q^{(*2)}$ depend on the shape of the inclusions (i.e., ellipsoid aspect ratio α), and are functions of the effective moduli and the moduli of phase 2. For spherical inclusions of phase 2, they are given by:

$$P^{(*2)}(y) = \frac{K^*(y) + \frac{4}{3}\mu^*(y)}{K_2 + \frac{4}{3}\mu^*(y)} \tag{3}$$

$$Q^{(*2)}(y) = \frac{\mu^*(y) + F^*(y)}{\mu_2 + F^*(y)} \tag{4}$$

where

$$F^*(y) = \frac{\mu^*(y)[9K^*(y) + 8\mu^*(y)]}{6[K^*(y) + 2\mu^*(y)]}. \tag{5}$$

Expressions for other ellipsoidal inclusions [based on Eshelby (1957)] may be found in Berryman (1980). Norris (1985) and Avellaneda (1987) have shown that the DEM is realizable and therefore is always consistent with the Hashin-Shtrikman upper and lower bounds.

In the usual DEM model, starting from a solid initial host, a porous material stays intact at all porosities and only falls apart at the very end when $y = 1$ (100 percent porosity). This is because the solid host remains connected and therefore load bearing. From equations (1) and (2) we see that as $y \to 1$, the left hand side goes to zero; to satisfy the equation, on the right hand side, $K^* \to K_2$ and $\mu^* \to \mu_2$. (For dry porous materials $\mu_2 = 0$ and $K_2 \approx 0$). The point (K_2, μ_2) is sometimes called the *attractor*. From any initial (K_1, μ_1) at $y = 0$, the solution always tends to (K_2, μ_2) as $y \to 1$.

While DEM is a good model for certain materials such as glass foam (Berge et al., 1993) and oceanic basalts (Berge et al., 1992), most reservoir rocks have a ϕ_c significantly less than 1.0 and are not represented very well by the conventional DEM theory. We can easily modify the DEM model to incorporate percolation behavior at any desired ϕ_c by redefining the phase 2 end member. The inclusions are now no longer made up of pure fluid (the original phase 2 material) but are composite inclusions of the critical phase at ϕ_c with elastic moduli (K_c, μ_c). With this definition, y denotes the concentration of the critical phase in the matrix. The total porosity is therefore given by $\phi = y\phi_c$. Starting from (K_1, μ_1) at $\phi = 0$ $(y = 0)$, the solution always ends up at (K_c, μ_c) for $\phi = \phi_c$ $(y = 1)$. The computations are implemented by replacing $(K_2,\ \mu_2)$ by $(K_c,\ \mu_c)$ everywhere in equations (1)— (5). Integrating along the reverse path, from $\phi = \phi_c$ to $\phi = 0$, gives lower moduli as now the softer critical phase is the matrix. The moduli of the critical phase may be taken as the Reuss average value at ϕ_c of the pure end member moduli. For porosities greater than ϕ_c, the material is a suspension and is best characterized by the Reuss average (or Wood's equation).

Figure 1 shows normalized bulk moduli curves for the conventional DEM theory (percolation at $\phi = 1$) and for the modified DEM (percolation at $\phi_c < 1.0$) for a range of ϕ_c values. When $\phi_c = 1$, the modified DEM coincides with the conventional DEM curve. The shapes of the inclusions were taken to be spheres in all cases. The path was from 0 to ϕ_c and (K_c, μ_c) were taken as the Reuss average values at ϕ_c. For this choice of (K_c, μ_c), estimates along the reversed path coincide with the Reuss curve. Since the critical phase consists of grains just barely touching each other, better estimates of K_c and μ_c may be obtained from measurements on loose sands or from models of granular material.

The elastic properties of the granular, unconsolidated critical phase are dominated by grain-to-grain contact interactions. Models of granular media express the effective elastic moduli of grain packs in terms of normal and tangential contact stiffnesses between grains, D_n and D_t respectively. For a brief review of contact theories see chapter 1 in Wang and Nur (1992). Walton (1987) gives the effective moduli for a random packing of identical elastic spheres, when they are infinitely rough (non-slipping contacts) or perfectly smooth (slipping contacts). Digby's (1981) model incorporates contacts initially bonded across a small circular area of radius b. The total contact area increases with increasing hydrostatic pressure and depends on the initial bonded radius. A number of variations on the type of contacts have also been presented (e.g. Yoshioka and Scholz, 1989; Goddard, 1990).

In our modeling we used Walton and Digby's theories [equation 4.10 in Walton (1987), and equations 33 and 34 from Digby (1981)], in addition to laboratory data, to get estimates of the critical phase moduli. We found that using (K_c, μ_c) from Digby's model as inputs to the modified DEM formulation gave reasonably good results. However, we do not claim that this is always the best estimate of the critical phase properties. Winkler (1983) showed that neither the conventional Hertz-Mindlin contacts nor the bonded Digby contacts predict D_n/D_t ratios that are consistent with laboratory data. Palciauskas (1992) has used Yoshioka and Scholz's (1989) rough contact model to calculate D_n/D_t ratios that agree well with laboratory observations. Though the ratio is easy to calculate, estimation of the actual effective moduli using the rough contact model requires several surface parameters that are usually difficult to determine. These include the asperity probability distribution function, the mean asperity curvature, and the asperity density. Better macroscopic descriptions of rough grain contacts as well as improvements in the packing models such as distributions of grain sizes and number of contacts are needed.

Comparison with Laboratory Data

Now we compare the modified DEM predictions with laboratory data on dry sandstones measured at ultrasonic frequencies. Figure 2 shows the dynamic bulk and shear moduli (circles and crosses, respectively) calculated from the measured velocities in clean sandstones (no clay) under 5 MPa confining pressure (Han, 1986). The solid and dashed curves represent the bulk and shear predictions, respectively. We see that the theory models the data reasonably well. The mineral moduli at $\phi = 0$ were those of quartz: $K_1 = 38$ GPa, and $\mu_1 = 44$ GPa. The critical phase end point (K_c, μ_c) was obtained from ultrasonic velocity measurements on unconsolidated, loose Ottawa sand, also at 5 MPa confining pressure (Yin, 1992) before the sand was subjected to pressure cycling. The critical porosity, $\phi_c = 0.387$, is the porosity of the loose sand. Bulk and shear moduli calculated from Walton's (1987) (infinitely rough spheres) and Digby's (1981) sphere pack model are also plotted on the figure and would likewise be good estimates for the critical phase properties. For the Digby model the ratio of initial bonding radius to grain radius, b/R, was taken as 0.01. The path of integration was from $\phi = 0$ to $\phi = \phi_c$. Calculations along the reversed path give lower moduli and do not fit the data very well. We found no obvious reasons why the rock at 6 percent porosity lies below the general trend. Since the presence of compliant, crack-like soft porosity tends to decrease the stiffness, perhaps this sample was more cracked than the others, causing its moduli to lie below the trend.

Figure 3a shows experimental and theoretical bulk moduli for sandstones under 40 MPa confining pressure. The data includes clean and clay-bearing sandstones (with up to 10 percent clay) from Han (1986) and Jizba (1991). The bulk moduli have been normalized by the mineral bulk modulus. For the clean sandstones, the mineral moduli at $\phi = 0$ were those of quartz; for the clay-bearing ones, the mineral moduli were obtained from the zero porosity intercept of Han's (1986) linear regression for shaly sandstones ($K_1 = 31$ GPa, $\mu_1 = 34$ GPa). Figure 3b is a similar plot for the shear modulus. In this case, the modified DEM estimates using (K_c, μ_c) obtained from Walton's theory or from data on Ottawa sand do not fit the data as well as at 5 MPa. The slightly stiffer critical phase moduli calculated from Digby's (1981) sphere pack model (with $b/R = 0.15$) give better results, though this b/R is somewhat high for a critical phase material. Digby's model considers the grains to be slightly cemented at their contacts. This stiffens the granular material and increases K_c and μ_c; perhaps this is more representative of the critical phase properties under high confining pressure. In fact, for these high pressure data, the modified Hashin-Shtrikman or even a straight line—the modified Voigt—captures the linear trend of the observations quite well (Yin et al., 1993).

Summary

Seismic velocities and elastic moduli of porous crustal rocks almost always show a percolation or critical porosity behavior. Below the critical porosity the rock is stiff and the solid frame is load bearing; above critical porosity the rock loses its cohesion and falls apart, behaving mechanically like a suspension. For most sedimentary rocks this percolation porosity is usually much less than 100 percent. The percolation behavior is a purely geometrical property, independent of physical properties of the rocks. Any valid velocity-porosity model for rocks must incorporate this critical porosity behavior and must also give estimates that always lie within the theoretically established bounds for elastic moduli. A simple way to include critical porosity as an input in existing analytical relations for two-phase composites is by redefining one of the end members to be the critical phase, and then renormalizing the porosity. We have shown how this simple concept can be used to modify the conventional DEM theory to have a percolation behavior at any desired critical porosity. The predictions of the modified DEM model compare favorably with ultrasonic laboratory data on sandstones. We have also suggested alternate ways of estimating the critical phase moduli which are used as one of the end members in the modified DEM equations. Since the DEM model has been proved to be realizable, the estimates are guaranteed to be always consistent with the Hashin-Shtrikman bounds.

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FIGURE CAPTIONS

Fig. 1. Normalized bulk moduli computed from the conventional DEM theory (percolation at $\phi = 1$) and from the modified DEM model (percolation at $\phi_c < 1$). The percolation porosity, ϕ_c, is the porosity at which the DEM curve meets the Reuss curve.

Fig. 2. Comparison of theoretical predictions with bulk and shear moduli (circles and crosses, respectively) obtained from ultrasonic measurements on dry sandstones under 5 MPa confining pressure (Han, 1986). The solid and dashed lines are the bulk and shear predictions, respectively. The end points for the theoretical curves at $\phi_c = 0.387$ are from loose sand data (Yin, 1992). Critical phase moduli computed from Walton's (1987) and Digby's (1981) sphere pack models are also plotted.

Fig. 3. a) Experimental and theoretical bulk moduli for sandstones under 40 MPa confining pressure. The experimental data are from Han (1986) and Jizba (1991). The moduli are normalized by the mineral bulk modulus end point at $\phi = 0$. The end points of the theoretical curves at the critical porosity are from the Digby (1981) sphere pack model. b) as in a) but for the shear moduli.