Velocity–porosity relationships: Predictive velocity model for cemented sands composed of multiple mineral phases

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ABSTRACT

Computer simulations are used to calculate the elastic properties of model cemented sandstones composed of two or more mineral phases. Two idealized models are considered – a grain-overlap clay/quartz mix and a pore-lining clay/quartz mix. Unlike experimental data, the numerical data exhibit little noise yet cover a wide range of quartz/cement ratios and porosities. The results of the computations are in good agreement with experimental data for clay-bearing consolidated sandstones.

The effective modulus of solid mineral mixtures is found to be relatively insensitive to microstructural detail. It is shown that the Hashin–Shtrikman average is a good estimate for the modulus of the solid mineral mixtures. The distribution of the cement phase is found to have little effect on the computed modulus–porosity relationships. Numerical data for dry and saturated states confirm that Gassmann’s equations remain valid for porous materials composed of multiple solid constituents. As noted previously, the Krief relationship successfully describes the porosity dependence of the dry shear modulus, and a recent empirical relationship provides a good estimate for the dry-rock Poisson’s ratio.

From the numerical computations, a new empirical model, which requires only a knowledge of system mineralogy, is proposed for the modulus–porosity relationship of isotropic dry or fluid-saturated porous materials composed of multiple solid constituents. Comparisons with experimental data for clean and shaly sandstones and computations for more complex, three-mineral (quartz/dolomite/clay) systems show good agreement with the proposed model over a very wide range of porosities.

1 INTRODUCTION

Developing accurate relationships between porosity and seismic wave velocities in porous rocks has been an important area of interest in rock physics for decades. Such relationships are crucial in relating in situ seismic/sonic measurements to porosity and fluid saturation. Present porosity–velocity relationships are based on theoretical formulae, rigorous bounds or empirical relationships.

Theoretical formulae are usually based on idealized morphologies; Wyllie’s time-average equation (Wyllie, Gardner and Gregory 1963), for example, is based on the assumption that pores and grains are arranged in homogeneous layers perpendicular to the seismic raypath. This equation and its underlying assumptions often lead to poor agreement with experiment. Effective-medium theories were developed to extend exact results for dilute inclusions to higher volume fractions. Some microstructures have been shown a posteriori to have properties that correspond to the theories, but the physical structures are very unusual and do not resemble those of porous rocks (Milton 1984).

Bounds are rigorously based on realistic microstructural information and are therefore widely applicable. Variational bounds include the simplest first-order bounds (e.g. Reuss and Voigt) and rigorous bounds based on expansions to third
order (Yeong and Torquato 1998). Bounds are particularly useful when they are narrow. However, when the moduli of two components differ significantly, the span of bounded properties becomes extremely large. Unfortunately this is the case for most porous rocks.

Empirical relationships remain most popular because they represent actual laboratory or log measurements. Unfortunately, measured porosity–modulus data usually display a high degree of scatter. This may be due to variations in lithology (pore shape, size, degree of compaction) (Marion et al. 1992) and, in particular, to clay content and distribution (Han 1986). Experimental data sets are therefore usually grouped into lithological types (see e.g. Nur et al. 1995; Wang 2000), such as dolostones, limestones, sandstone, shaly sands and shales. While useful for summarizing lithotypes, empirical relationships are limited by the scatter in the measured data sets and can seldom be applied successfully outside the range of the measured data.

In previous papers (Arns, Knackstedt and Pinczewski 2002a; Knackstedt, Arns and Pinczewski 2003), we have shown that it is possible to explore velocity–porosity relationships in a more precise way by computing the elastic properties of digital models of complex microstructures, where the microstructure and mineralogy of the material is known and where it is possible to average over a number of statistically identical samples. The computed data, although based on idealized microstructures, allow a quantitative analysis of the effects of porosity and the distribution of the mineral phases on the elastic properties of the model rocks. Our previous computational studies of modulus–porosity relationships were limited to clean (monomineral) rock systems. However, actual sandstones are rarely clean and often contain minerals other than quartz (e.g. clays), which can affect their elastic properties. Clay can be distributed in a number of ways in the rock framework depending on the conditions at deposition, on compaction, bioturbation and diagenesis. Most empirical relationships (e.g. Castagna, Batzle and Eastwood 1985; Han 1986; Han, Nur and Morgan 1986) and theoretical models (Xu and White 1995) account for the volume of clay present and ignore its distribution. An advantage of numerical models is that they can be used to study complex multiphase materials with physically realistic phase distributions. We consider two model distributions of cemented sandstone composed of two or more mineral phases: a grain-overlap model, where grains of cement are distributed structurally, and a pore-lining cementation model, where the cement phase develops uniformly on the original sand/pore interface. We study model clay/quartz and dolomitic/quartz cemented sands and use computer simulation to determine the elastic properties of the model systems. We generate porosity–moduli relationships for both the dry and water-saturated states for the model cemented sandstone morphologies. Since the pore space and the solid phase microstructure and mineralogy of the model systems are precisely defined, the resultant numerical data sets exhibit very little noise or scatter and it is possible to analyse porosity–modulus relationships quantitatively in the absence of experimental noise.

The effective moduli of the solid mineral mixtures show a small dependence on microstructure. We compare the numerically determined moduli of the solid mineral mixtures with effective-medium and empirical estimates and find that the Hashin–Shtrikman average provides a good estimate for the modulus of the solid mineral mixture. Weighted Hashin–Shtrikman fits (Wang, Wang and Cates 2001) are also presented.

We find that, for all porosities, the choice of a microstructural model for cementation has a minimal effect on the resultant modulus–porosity relationship. Gassmann’s equations are verified for the porous materials made up of multiple solid constituents. Agreement of the predictions with experimental data sets for clay-bearing consolidated sandstones is encouraging. As previously noted for clean sandstone systems (Knackstedt et al. 2003), the Krief empirical relationship (Krief et al. 1990) is found to be particularly successful in describing the porosity dependence of the shear modulus, and a recent empirical method (Arns et al. 2002a) provides a good prediction of the Poisson’s ratio data for dry rock.

From the computed results, we propose a new empirical model which describes the full modulus–porosity relationship for isotropic dry and fluid-saturated consolidated sand systems and requires only a knowledge of the mineral constituents and the proportion of each mineral phase present. The effective solid modulus of the mineral phase is given by the averaged Hashin–Shtrikman equation,

\[ M_{\text{eff}} = (M_1 + M_2)/2, \]  

where \( M \) denotes both the bulk (\( K \)) and shear (\( \mu \)) moduli and \( M_1 \) and \( M_2 \) are the Hashin–Shtrikman lower and upper bounds, respectively. The porosity dependence of the cemented sands follows the same empirical method proposed previously for clean sandstones (Krief et al. 1990; Arns et al. 2002a):

\[ \mu(\phi) = \mu_{\text{eff}}(1 - \phi)^{m(\phi)} \]  

and

\[ \nu_{\text{dry}}(\phi) = \alpha(\phi) + (1 - (2\phi)^{1/2})\nu_{\text{eff}}, \]
where \( \nu \) is Poisson’s ratio. Gassmann’s equations are subsequently used to determine the fluid-saturated states. Comparisons of the proposed method with the results of numerical simulations for systems containing as many as three individual mineral phases and with a number of experimental studies are encouraging.

2 MODEL ROCK SYSTEMS

2.1 Two-mineral-phase microstructure

In a previous study we generated idealized single-mineral model rock morphologies over a very wide range of porosities using a simple Boolean overlapping spheres model (Knackstedt et al. 2003). In the present study we extend this idealized model to two-mineral phases in which the second mineral is either randomly dispersed via grain overlap throughout the medium (Fig. 1) or distributed as a uniform pore-lining phase around the first mineral (Fig. 2). A wide range of porosities and mineral ratios are realized by varying the number of spheres and the thickness of the pore-lining phase.

We report the ratio of the mineral phases (\( M_1:M_2 \)) along with the order of placement, mineral-1 then mineral-2, and the porosity. For example, a quartz/clay grain-overlap model microstructure at a 2:1 ratio is generated by placing quartz spheres to a predetermined volume fraction, then placing identical spheres of clay phase on to the quartz/pore mixture until the required volume ratios of both mineral phases and porosity are reached. Boolean statistics (see e.g. Arns et al. 2001) allow model systems to be generated with the specified phase fractions by relating the density of the spheres directly to the volume fraction of the phase – if spheres of volume \( V_s \) are placed with probability \( \mu \), then the porosity \( \phi \) of the final configuration is given by

\[
\phi(\mu) = e^{-\mu V_s}.
\]

(4)

Equations for multiphase materials are easily derived in a completely analogous manner. We consider a number of mixtures over the porosity range \( 0 < \phi < 0.5 \). We consider quartz as \( M_1 \) and both clay and dolomite as the second \( M_2 \) phase at ratios 1:1, 2:1 and 4:1. We also consider the reverse systems: clay or dolomite placed first with quartz grain overlap at volume ratios of 1:1, 2:1 and 4:1. Examples of the microstructure of the grain-overlap model at different mineral ratios and porosities are illustrated in Fig. 1.

In the uniform pore-lining model, we begin with an overlapping-spheres model for the first mineral phase; spheres of \( M_1 \) are placed until the required volume fraction of that
Figure 2 Slices through the pore-lining two-phase mineral model at the resolution used in the elastic simulations (120³). Top row: M₁:M₂ ratio of 1:1; second row: M₁:M₂ ratio of 2:1; bottom row: M₁:M₂ ratio of 4:1. The volume fractions of the three phases (M₁,M₂,φ) in (a)–(i) are the same as in Fig. 1.

mineral phase is reached. The second mineral phase M₂ is then developed by allowing parallel surfaces originating from the grain/pore interface of the original spheres to grow into the pore space. Examples of the model microstructure are given in Fig. 2. The model is similar to the model previously considered by Dvorkin and Nur (1996). Neither the grain-overlap nor the pore-lining models are limited to spherical particles. Both are readily extended to any type of spheroidal shape. Computations for isotropic packings of more complex spheroidal particles and mixtures of varying packings yield similar results to those reported here. In this paper, we do not consider globally anisotropic packings of complex systems, which are important in the consideration of shaly sandstones (Hornby, Schwartz and Hudson 1994).

As described previously (Arns et al. 2002a,b; Knackstedt et al. 2003), we use a finite-element method (Garboczi and Day 1995) to calculate the elastic properties of the model systems. Each data point represents a minimum of 10 independent simulations to reduce statistical errors. The simulations were run on several nodes of a Compaq ES40 supercomputer over a period of months. Approximately two years of workstation time was required to perform the simulations described here. The mineral properties used are shown in Table 1 (Mavko, Mukerji

<table>
<thead>
<tr>
<th></th>
<th>K (GPa)</th>
<th>µ (GPa)</th>
<th>ρ (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>37.0</td>
<td>44.0</td>
<td>2.65</td>
</tr>
<tr>
<td>Dolomite</td>
<td>69.4</td>
<td>51.6</td>
<td>2.70</td>
</tr>
<tr>
<td>Clay</td>
<td>20.8</td>
<td>6.9</td>
<td>2.60</td>
</tr>
<tr>
<td>Water, T = 200° C, 40 MPa</td>
<td>2.2</td>
<td>0.0</td>
<td>1.00</td>
</tr>
</tbody>
</table>

and Dvorkin 1998). The choice of the water-saturated condition is made to allow for comparison with experimental data from Han (1986).

3 RESULTS

3.1 Effective mineral modulus of two-phase material

We first consider the effect of mineral distribution on the resultant moduli (Kₑₑ, µₑₑ) of a solid two-phase mixture (φ = 0). The results are summarized in Fig. 3. When the elastic properties of the individual minerals are similar, bounds can be used to predict the effective elastic properties of multiphase mixtures with high accuracy. We use bounds to test the accuracy
of the numerical results. The data in Fig. 3 include predictions for the Hashin–Shtrikman lower \((K_s, \mu_s)\) and upper \((K_u, \mu_u)\) bounds for comparison with the numerical data. All numerically derived data points lie within the bounds, even when the bounds are very tight (quartz/dolomite system, Q:D).

The computed values of bulk and shear moduli for the grain-overlap and pore-lining models are similar, indicating only a small dependence of the moduli on microstructure or the distribution of the second mineral phase. The shear modulus for the quartz/clay system displays the largest dependence on microstructure: \(\pm 10\%\) difference in \(\mu_{\text{eff}}\) for the two different microstructures. This is due to the large contrast between the properties of the two phases \((\mu_{\text{quartz}} = 44.0, \mu_{\text{clay}} = 6.9)\). The contrast in property values for the other systems is considerably smaller, less than a factor of two, and the resultant moduli can be considered to be essentially independent of structure.

We also observe differences in the modulus for the quartz/clay system (Q:C) when the order of mineral placement is reversed. For example, \(\mu_{\text{grain}}\) (Q:C = 1:1) = 18.6, while \(\mu_{\text{grain}}\) (C:Q = 1:1) = 16.9 for the grain-overlap model. Similar differences are observed for the pore-lining model, where \(\mu_{\text{pore}}\) (C:Q = 1:1) = 17.0 > \(\mu_{\text{pore}}\) (Q:C = 1:1) = 18.7. The differences in modulus values are directly related to the difference in connectivity of the phases. When the stiffer phase (quartz) exhibits enhanced connectivity, the effective modulus is greater. The grain-overlap model displays higher interconnectivity for the phase placed first (see Fig. 1). For the pore-lining model, the second mineral phase, developed by parallel surfaces, is the more highly interconnected phase (see Fig. 2).

### 3.2 Dry rock

Figures 4–6 show results for dry bulk modulus \(K\), shear modulus \(\mu\), compressional velocity \(V_p\) and compressional/shear velocity ratio \(V_p/V_s\) for the model systems as a function of porosity for different sand/cement ratios, i.e. 1:1 (Fig. 4), 2:1 (Fig. 5) and 4:1 (Fig. 6). The standard error is plotted to show the quality of the numerical data. For \(K, \mu\) and \(V_p\), the standard errors are always smaller than the symbols used to represent the actual data points. The standard error for the \(V_p/V_s\) ratio is small for porosities \(\phi < 0.2\) but increases at higher porosities. This is particularly evident for the 1:1 mineral ratio results (Fig. 4d). However, the overall trend in the numerical data remains clear.

The moduli all trend from the effective modulus for the mineral mixture at low porosities to zero at higher porosities. The fit to the numerical modulus data is, for most cases, highly non-linear, with a critical porosity where the modulus vanishes at \(\phi \approx 0.5\). In all cases the moduli for the quartz/dolomite systems exhibit little dependence on microstructure. The moduli of the quartz/clay systems show a small dependence on microstructure. For example, the grain-overlap model for the quartz/clay system has a larger bulk modulus than the corresponding pore-lining model. The difference between the two models, which was reflected in the moduli of the solid phase (see Fig. 3), is again due to the better interconnectivity of the quartz phase in the grain-overlap model, where quartz has the higher modulus.

Figures 4–6 show that the \(V_p\) curve is approximately linear with porosity. The \(V_p/V_s\) ratio displays a non-linear dependence on porosity and tends to a fixed value \((V_p/V_s)^\ast \approx 1.63 = \sqrt{(8/3)}\) at high porosities. This behaviour was noted previously (Arns et al. 2002a) and corresponds to a Poisson’s ratio \(v^\ast(\phi = 0.5) = 0.2\). The behaviour is similar to that theoretically derived in two dimensions (Cherkaev, Lurie and Milton 1992; Day et al. 1992).

### 3.3 Water-saturated rock

Figures 7–9 show computed water-saturated values for the bulk modulus \(K\), shear modulus \(\mu\), \(V_p\) and \(V_p/V_s\) ratio for the model systems as a function of porosity. The standard error is also plotted. Again, the standard error is in most cases smaller than the size of the symbols used to represent the data points. Data for the moduli display qualitative behaviour similar to that for the previously discussed dry-rock case. The bulk moduli for the models now trend non-linearly between the modulus of the mineral at zero porosity to values corresponding to a
mineral-pore suspension at large $\phi$. The shear moduli show the same behaviour as that for the dry rock, tending to zero at higher porosities. In most cases, the dependence of the moduli on the distribution of the cemented phase (microstructure) is even smaller than that for the dry systems (Figs 4–6).

The saturated $V_p/V_s$ ratios exhibit a stronger dependence on microstructure and mineralogy than those for the corresponding dry systems. The 1:1 clay/quartz system (Fig. 7d) displays a difference between the behaviour of the grain-overlap and pore-lining models. The difference is greater for the 4:1 ratio quartz/clay system (Fig. 9d). The saturated $V_p/V_s$ ratio data is reasonably independent of the distribution of the cemented phase for $\phi < 0.2$. Large differences are observed at higher porosities.

3.4 Verification of Gassmann’s equation for multiple mineral phases

The low-frequency Gassmann’s equations relate the bulk and shear moduli of a saturated porous medium to the moduli of the corresponding dry state. For an isotropic monomineral medium, Gassmann’s relationships allow the prediction of the effective bulk modulus $K_{sat}$ for the saturated rock from knowledge of the dry frame modulus $K_{dry}$ and the pore-fluid modulus $K_f$:

$$\frac{K_{sat}}{K_0 - K_{sat}} = \frac{K_{dry}}{K_0 - K_{dry}} + \frac{K_f}{\phi(0 - K_f)},$$

(5)

where $\phi$ is the porosity. Gassmann’s relationships show that the shear modulus is mechanically independent of the
properties of the fluid in the pore space, i.e.
\[ \mu = \mu_{\text{sat}}. \]  \hfill (6)

Gassmann's relationships, (5) and (6), assume that the porous medium contains only one solid constituent with a homogeneous mineral modulus, that the pore space is statistically isotropic and that frequencies are low; conditions are quasistatic so that induced pore pressures are equilibrated throughout the pore space. The low-frequency limit coincides with the conditions for the finite-element approach used here. We find that the numerical data for the multimineral model also obey Gassmann's relationships for all ratios of minerals. Figure 10 shows this for both the grain-overlap and pore-lining models at a 2:1 mineral ratio. The numerical data for both the bulk and shear moduli are in excellent agreement with Gassmann's relationships.

### 3.5 Comparison with experiment

#### 3.5.1 Dry rock

Han (1986) reported experimentally measured elastic properties for 69 sandstone samples with different porosities and clay volume fractions \( C \). For clarity, we have divided these data into five groups based on clay content: clean \((C = 0)\), intermediate \((0 < C < 0.1)\), mid-range \((0.1 < C < 0.2)\), high \((0.2 < C < 0.35)\) and extreme \((0.35 < C < 0.5)\). To compare the measured data with simulations, we relate the total clay concentration \( C \) to clay solid fractions, \( X_c \), using \( C = X_c \times (1 - \phi) \). We define a mean \( X_c \) within each of the five groups by averaging over the porosities within each experimental data group: clean \( (X_c = 0) \), intermediate \( (X_c \approx 0.07) \), mid-range \( (X_c \approx 0.2) \), high \( (X_c \approx 0.3) \) and extreme \( (X_c \approx 0.5) \). Since the differences between the elastic properties computed with the
Dvorkin and Nur (1996) reported bulk and shear moduli and Poisson's ratio ($V_p/V_s$) measurements for high porosity $\phi = 0.2–0.35$ core plugs from the Oseberg field. The samples are predominantly quartz, bound by quartz and clay cements. Clay volume fractions ranged from 0.1 to 0.25. They modelled the Oseberg sandstone as hard-shell quartz grains with cement uniformly deposited on the grain surfaces. Calculations based on an effective-medium approach produced results which were in reasonable agreement with the measured moduli but the match for Poisson's ratio was poor. Our pore-lining model, discussed above, is very similar to this model and we therefore compare the Oseberg data with computations performed using the pore-lining model. For the purposes of comparison, we consider the cases of a clean sandstone and a clay-bearing sand with $X_c = 0.33$. These two cases represent upper and lower bounds for the experimental data. The comparison is shown in Fig. 12. The computed bounds for the moduli data are reasonable. The computed bounds for the $V_p/V_s$ data are poorer but are considerably better than those obtained by Dvorkin and Nur (1996), who proposed that $V_p/V_s \simeq 1.45$.

Wang (2000) recently reported a set of correlations relating $V_p$ and $V_s$ to bulk densities for a number of lithologies including quartz sandstones with clay content $0 < C < 0.15$ and for shaly sandstones – quartz sandstones with clay content.
Velocity–porosity relationships

Figure 7 Comparison of simulations for water-saturated bulk modulus, shear modulus and $V_p/V_s$ ratio for the model cemented sands at a 1:1 mineral ratio. Symbols/lines are the same as in Fig. 4.

$0.15 < C < 0.6$. The correlations in units of km/s were written as,

\[ V_p = a_p + b_p \rho, \]  
\[ V_s = a_s + b_s \rho, \]  
\[ V_p = c_p \rho^{d_p}, \]  
\[ V_s = c_s \rho^{d_s}. \]

The values of the constants are given in Wang (2000).

In order to compare our computations with the correlations, we assume that the modulus properties of gas-saturated rocks are the same as our predictions for the dry modulus and that the ideal gas law can be used to estimate $\rho_{\text{gas}}$ (40 MPa) = 0.226 g/cm$^3$. We compare the correlations for clean sands with our computed data for pure quartz sands (Knackstedt et al. 2003) and for cemented sands with a quartz/clay ratio of 4:1 (Fig. 13a,b). The computed points provide good upper and lower bounds for the empirical correlations. Similar comparisons of the correlations for shaly sandstones to computed data with quartz/clay ratios of 4:1 and 1:1 are shown in Fig. 13(c,d). Again, the computed data points give approximate upper and lower bounds for the correlations, however, the slope of the computed points is different from that of the correlations. This may be due to the fact that higher density (lower porosity) rocks tend to be more clay-rich. This may explain why the correlations (Wang 2000) trend between the high clay predictions (diamonds) at high densities towards the lower clay-content prediction (squares) at low densities.
Figure 8 Comparison of simulations for water-saturated bulk modulus, shear modulus and $V_p/V_s$ ratio for the model cemented sands at a 2:1 mineral ratio. Symbols/lines are the same as in Fig. 4.

3.5.2 Water-saturated rock

Figure 14 shows a comparison between the experimental data of Han (1986) for water-saturated rocks, divided into five groups based on clay content, and computations for clean quartz (Knackstedt et al. 2003) and for clay-cemented quartz sands with the same range of quartz/clay fractions ($0 < X_c < 0.5$). The agreement between the computations and the measured data is encouraging.

Han (1986) also reported empirical correlations based on least-squares fits to his measured data. His correlations for water-saturated sandstone velocities (in km/s) at a confining pressure of 40 MPa over a wide range of porosities ($0.05 < \phi < 0.3$) and clay contents ($0 < C < 0.5$) are

\[ V_p = 5.59 - 6.93\phi - 2.18C \]  \hspace{1cm} (11)

and

\[ V_s = 3.52 - 4.91\phi - 1.89C. \]  \hspace{1cm} (12)

We compare the above correlations with our computations by transforming (11) and (12) from $V_p(\phi, C)$ to $V_p(\phi, X_c)$. Figure 15 shows that the agreement between the empirical correlations and the computations is good for $V_p$ but overpredicts $V_s$ at intermediate clay fractions.

We also compare Han’s (1986) correlations for clean sandstone data,

\[ V_p = 6.08 - 8.06\phi \]  \hspace{1cm} (13)

and

\[ V_s = 4.06 - 6.28\phi. \]  \hspace{1cm} (14)
with the numerical model. The comparison is shown in Fig. 15. The agreement is excellent for both $V_p$ and $V_s$.

A number of correlations relating $V_p$ to $V_s$ have also been reported. Castagna, Batzle and Kan (1993) provided the following correlation for clean sandstones:

$$V_s = 0.804 V_p - 0.856. \quad (15)$$

Han (1986) provided a correlation for shaly sandstones with different clay volumes:

$$V_s = 0.754 V_p + 0.57, \quad C < 0.25, \quad (16)$$

and

$$V_s = 0.842 V_p + 1.099, \quad C > 0.25. \quad (17)$$

The mudrock line of Castagna et al. (1993) is almost identical to (17). Figure 16 shows a comparison between the above correlations and our computations. The agreement between the computations and the empirical correlations is good. The numerical predictions for clean and shaly sandstones all collapse to a straight line as is observed experimentally. The numerical predictions indicate that, in accordance with the empirical correlations, $V_s$ decreases slightly with increasing clay content at constant $V_p$.

Finally, we compare the correlations developed by Wang (2000) for water-saturated $V_p$ and $V_s$ as a function of bulk densities, for clean and shaly sands (see equations (7)–(10)) with the numerical computations. The comparison is shown in Fig. 17. The deviations between the empirical linear and non-linear fits can be extensive and the computational data lie

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Figure 10 Comparison of simulations for dry and water-saturated model morphologies at a 2:1 mineral ratio. (a) and (b) show data for the grain-overlap model, (c) and (d) for the pore-lining model. In (a) and (c), dry data are represented by open symbols and wet by full symbols. The solid lines show the best fit to the dry data. Gassmann’s relationship (5) is used to predict the water-saturated bulk modulus based on the fit to the dry-rock data and this result is shown by the dashed lines. (b) and (d) show that the shear modulus is independent of the pore fluid as predicted by (6).

The agreement is best for the cleaner sands. Also shown in Fig. 17(a) is a comparison between our computations and the relationships of Gardner, Gardner and Gregory (1974) and the more recent correlations of Wang (2000). The more recent correlations are in better agreement with the numerical model.

The encouraging overall agreement between the computations for the model systems and available measured data for clean and shaly sandstones suggests that the models provide a good representation of the behaviour of consolidated sandstones and confirms the utility of the numerical data sets.

4 COMPARISON WITH MODELS

Relatively simple theoretical models and empirical relationships have been used to describe the mechanical properties of complex sedimentary rock. In this section, we compare a selection of these models with the results of the computations discussed in the previous section.

4.1 Effective mineral properties

All moduli–porosity relationships require the moduli of the solid mineral mixture to be specified. While the moduli of
Figure 11 Comparison of $V_p$ and $V_s$ data of Han (1986) divided into five groups based on clay fraction ($0 < X_c < 0.5$) and simulations for clean sand and shaly sands with clay contents $X_c = 0, 0.33$ and 0.5.

Figure 12 Comparison of the experimental data of Dvorkin and Nur (1996) for high-porosity Oseberg sandstone with clay volume fractions $C = 0.1–0.25$ and simulations for clean sand, $X_c = 0$, and shaly sands with a clay solid fraction, $X_c = 0.33$.

pure mineral phase is known, the effective modulus for a mineral mixture is not. In this section, we first compare the solid moduli obtained numerically for mixed lithologies to two theoretical effective-medium theories (the self-consistent method (SCM) and the differential effective medium (DEM)) and to three empirical estimates: the Voigt–Reuss–Hill (VRH) estimate, the averaged Hashin–Shtrikman (HS) estimate and the geometric average of velocities used by Xu and White (1995) (XW). The two effective-medium theories are described in detail by Berryman (1995), and discussions can be found in several texts (see e.g. Mavko et al. 1998). The Voigt–Reuss–Hill estimate is simply the arithmetic average of the Voigt upper bound ($M = \sum_{i=1}^{N} f_i M_i$) and the Reuss lower bound ($M = \sum_{i=1}^{N} f_i / M_i$) where $f_i$ and $M_i$ are the volume fraction and the moduli of the $i$th component. Similarly, the Hashin–Shtrikman average is the average of the upper and lower Hashin–Shtrikman bounds (Mavko et al. 1998). Xu and White (1995) estimated the velocities of a solid mineral mixture in shaly sands using a Wyllie time-average equation of the quartz and clay mineral velocities and an arithmetic average of their densities.

A comparison between the predictions of the above five methods and our computations is given in Table 2. For the Xu and White (1995) method, predictions for $M$ are only given for shaly sands (quartz/clay) mixtures as this estimate was derived specifically for these systems. All the predictions for the quartz/dolomite systems are within $\pm 2\%$ of the computed data. This is well within the order of the standard error for the computations. The numerical data do show some significant deviations from the theoretical model predictions for the quartz/clay systems where the contrast between the individual mineral moduli is higher. For these cases we find that the self-consistent method, the differential effective-medium predictions, the Voigt–Reuss–Hill and Hashin–Shtrikman average estimates show deviations. No consistency with model morphologies is observed. The empirical method of Xu and White...
If we define systems, not by model type, but by the preferred connectivity or continuity of the stiffer or weaker phase, we observe a more consistent trend in the data. As discussed previously, for the grain-overlap model, the connectivity of the phase placed first is higher (see Fig. 1). For the pore-lining model, the connectivity of the second mineral phase, developed by parallel surfaces, is higher (see Fig. 2). We therefore plot the data for the models where the stronger and weaker phases – quartz and clay, respectively – preferentially form the most highly interconnected structure as a function of clay content. We plot the relative error in the predictions for the bulk and shear moduli for the four models where $\text{Error} = (M_{\text{model}} - M_{\text{sim}})/M_{\text{sim}}$. In Fig. 18(a,b) for the case where the quartz (stiffer) phase is preferentially connected, we observe that the models consistently underestimate the moduli. Figure 18(c,d) shows that when the clay (weaker) phase is preferentially connected, the moduli are overestimated. We conclude that the self-consistent method and the averaged Hashin–Shtrikman bounds perform the best.

Hashin–Shtrikman bounds require only knowledge of the volume fractions of the mineral components. Better predictions for the effective moduli of two-phase quartz/clay mineral
Figure 14 Comparison of computed water-saturated $V_p$ and $V_s$ with experimental data of Han (1986) for a wide range of clay fractions.

Figure 15 Comparison of the empirical equations (11)–(14) of Han (1986) with numerical simulations. The simulation data match very well for all $V_p$ data but overestimate the empirical prediction for $V_s$. The numerical predictions for clean sandstone match the empirical results well.

mixtures could be obtained using higher-order bounds. Unfortunately, this requires information in the form of three-point statistical correlations (Yeong and Torquato 1998), which is difficult to obtain experimentally.

An improved method described by Wang et al. (2001) is based on a primitive knowledge of phase distribution and the weighted Hashin–Shtrikman average. Using the knowledge that if the stiffer component forms the primary backbone of the two-component material, the real values of the effective moduli are closer to the upper Hashin–Shtrikman bound and if the weaker material forms the more highly connected backbone, the effective moduli are closer to the lower Hashin–Shtrikman bound, Wang et al. (2001) gave estimates for the effective moduli from the Hashin–Shtrikman lower and upper bounds ($K_l$, $\mu_l$ and $K_u$, $\mu_u$) using the relationships,

$$K_{\text{eff}} = a K_u + (1 - a) K_l$$

and

$$\mu_{\text{eff}} = b \mu_u + (1 - b) \mu_l,$$

where $a$ and $b$ are empirical weights defined as Hashin–Shtrikman coefficients. Wang et al. (2001) determined $a$ and $b$ experimentally by performing measurements on an epoxy/clay mixture, where the epoxy (softer material) was the continuous phase and the clay (stiffer material) was dispersed within the epoxy resin. They found that the Hashin–Shtrikman

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coefficients were small \((a, b < 0.5)\) and exhibited a clear
dependence on the epoxy concentration \(c\), i.e. \(a = 0.37 - 0.27c\)
and \(b = 0.33 - 0.2c\). The lower bounds were used because
the softer epoxy material formed the continuous phase.

We use the above method to obtain estimates for the
effective moduli of the mixed mineral systems. The Hashin–
Shtrikman coefficients for the bulk and shear moduli are sim-
ilar and can be approximated by \(a, b \simeq 0.7(1 - c); 0.2 < c < 0.8\) for the case where clay is the more continuous phase
and \(a, b \simeq (1 - 0.8c); 0.2 < c < 0.8\) when quartz is the more
continuous phase. The qualitative shift in the coefficients with
clay content noted by Wang et al. (2001) is consistent with the
numerical data. We note that the epoxy/clay mixtures in Wang
et al. (2001) give smaller values for \(a\) and \(b\), but in that case
the stiffer phase is completely unconsolidated.

In general, the average Hashin–Shtrikman prediction pro-
vides a good prediction of the moduli; however, if the contin-
unity of the stiffer/weaker phase can be ascertained, one could
weight the bounds to higher/lower values. We use the simple
average Hashin–Shtrikman prediction for all estimates made in
the remainder of this paper.

4.2 Dry rock

In a previous paper (Knackstedt et al. 2003), we compared
computed data with a number of theoretical methods includ-
ing Hashin–Shtrikman bounds and effective-medium theories
(both the self-consistent method and the differential effective
medium). For monomineral systems, we found that none of
the theoretical methods provides an acceptable fit to the data.
We make the same conclusions for the model cemented sands
considered here although we do not show the data (for repre-
sentative curves see figs 10 and 14 of Knackstedt et al. (2003)).
In all cases, bounds and the self-consistent method and differ-
tential effective-medium theories overestimate the numerical
data for both dry and water-saturated systems. As previously
noted (Berge, Berryman and Bonner 1993), the self-consistent
method theory gives the best agreement with data. In this sec-
tion we compare results of the more common empirical equa-
tions with our numerical data.

If dry rock is modelled as an elastic porous solid, the dry-
rock bulk modulus may be written as \(K_{dry} = K_0(1 - \beta)\), where
\(\beta\) is Biot’s coefficient. Krief et al. (1990) used experimental
data to find the following empirical relationship for \(\beta\) as a
function of \(\phi\): \(1 - \beta = (1 - \phi)^m(\phi)\) where \(m(\phi) = 3/(1 - \phi)\).
They used the empirical result of Pickett (1963) which assumes
that the dry-rock Poisson’s ratio is approximately equal to the
mineral Poisson’s ratio, or \(\mu_{dry}/K_{dry} = \mu_0/K_0\), which leads to
\[
K_{dry} = K_0(1 - \phi)^m(\phi) \quad (20)
\]
and
\[
\mu_{dry} = \mu_0(1 - \phi)^m(\phi). \quad (21)
\]
Nur et al. (1995) proposed similar linear modulus–porosity
relationships with a critical porosity:
\[
K_{dry} = K_0 \left(1 - \frac{\phi}{\phi_c}\right) \quad (22)
\]
and
\[
\mu_{dry} = \mu_0 \left(1 - \frac{\phi}{\phi_c}\right), \quad (23)
\]
where the critical porosity \(\phi_c\) for sandstones was empirically
found to be 0.40 for both sands and shaly sands (Nur, Marion
and Yin 1991). Comparisons between both empirical models
and computed data for the pore-lining model morphology are
shown in Fig. 19. The results are mixed. The computed data
clearly display a non-linear relationship between moduli and
porosity which the prediction of Nur et al. (1995) fails to cap-
ture. The result of Krief et al. (1990) (equation (21)) provides
a reasonable estimate for the bulk modulus and is particularly
accurate for the shear modulus.

Figures 4(d), 5(d) and 6(d) show the computed data for the
\(V_p/V_s\) ratio for the dry-rock case. The models of both Krief
et al. (1990) and Nur et al. (1995) assume \(\frac{V_p}{V_s}\)_{dryrock} = \(\frac{V_p}{V_s}\)_{mineral}. These predictions are clearly a poor match to the

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Numerical data. Arns et al. (2002a) recently reported similar limiting behaviour for Poisson's ratio for porous granular models and derived a very accurate empirical equation for Poisson's ratio of dry porous materials:

$$v_{\text{dry}} = a(\phi) + v_s(1 - 2\phi)^{3/2},$$  \hspace{1cm} (24)

where $a(\phi) = (2\phi)^{3/2}/5$, for $v_s < 0.2$, and $a(\phi) = 1 - (1 - 2\phi)^{3/2}/5$, for $v_s > 0.2$. The relationship for $V_p/V_s$ is given by

$$V_p/V_s = \sqrt{\frac{\nu - 1}{\nu - 0.5}}.$$  \hspace{1cm} (25)

Figure 20 shows a comparison between the above empirical model and the computed numerical data for $V_p/V_s$. The agreement with the computed data is good for all systems and is clearly superior to the assumption that $(V_p/V_s)_{\text{dry rock}} = (V_p/V_s)_{\text{mineral}}$.

### 4.3 Water-saturated rock

Measurements by Wyllie et al. (1956, 1958, 1963) show that the sonic velocities of water-saturated sedimentary rocks having relatively uniform mineralogy may be related to porosity by simple monotonic relationships. They expressed these relationships as

$$\frac{1}{V_p} = \frac{\phi}{V_{pf}} + \frac{1 - \phi}{V_{ps}},$$  \hspace{1cm} (26)
Table 2  Dry moduli for the mixed lithologies at zero porosity for the grain-overlap model ($K_{\text{grain}}$, $\mu_{\text{grain}}$) and the pore-lining model ($K_{\text{porelin}}$, $\mu_{\text{porelin}}$) in GPa. The comparison with the averaged Hashin–Shtrikman prediction $K_{\text{HS}}$, the Voigt–Reuss–Hill average $K_{\text{VRH}}$ and predictions based on the self-consistent method $K_{\text{SCM}}$ and differential effective medium $K_{\text{DEM}}$ are satisfactory for most systems. Only the shear modulus data for the quartz/clay system where the modulus difference between the two phases is more than a factor of 7 give a poorer prediction. The error in this case is up to 10%. The predictions of the time-average equation $K_{\text{XY}}$ (Xu and White 1995) are poor.

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<th>$K_{\text{VRH}}$</th>
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Raymer, Hunt and Gardner (1980) suggested the following improvements to Wyllie’s empirical relationship:

\[ V_p = (1 - \phi)^2 V_{ps} + \phi V_{pf}, \quad \phi < 0.37, \]

\[ \frac{1}{\rho V_p^2} = \frac{(1 - \phi)}{\rho_s V_{ps}^2} + \frac{\phi}{\rho_s V_{pf}^2}, \quad \phi > 0.47, \]

\[ \frac{1}{V_p} = 0.47 - \frac{\phi}{0.10 \times V_{37}} + \frac{\phi - 0.37}{0.10 \times V_{47}}, \quad 0.47 > \phi > 0.37, \]

where $V_{37}$ is calculated from the low-porosity formula at $\phi = 0.37$ and $V_{47}$ is calculated from the high-porosity formula at $\phi = 0.47$.

Figure 21 shows a comparison between the sonic velocities computed for the pore-lining model for mineral ratios of: (a) 1:1, (b) 2:1 and (c) 4:1. In most cases the Raymer equation produces a much better fit to the numerical data than the Wyllie equation. However, the Raymer equation consistently underestimates the numerical data for $V_p$ for $\phi < 0.35$. The Raymer equation shows the experimentally observed transition from the load-bearing domain to the suspension domain at $\phi \geq 0.37$. While both the grain-overlap and pore-lining models display a small shift in the $V_p$ curve at $\phi \approx 0.35–0.4$, the shift is not as dramatic as that for the empirical Raymer equation. As explained previously, this is the result of the choice of the microstructural model – a model based on permeable spheres – which is clearly not realistic for porosities $\phi > 0.35$ because the model structure remains load-bearing.

5 A NEW PREDICTIVE VELOCITY MODEL FOR CEMENTED SANDS

Based on the particular success of some of the empirical and theoretical relationships discussed in Sections 3 and 4, we propose a new empirical predictive model for the full modulus–porosity relationship for a consolidated granular system in dry and saturated states. The model is based solely on knowledge of the mineral constituents and the proportion of each mineral phase present.

The effective solid modulus of the mineral phase is given by the averaged Hashin–Shtrikman equation,

\[ M_{eff} = (M_1 + M_0)/2, \]

where $M$ denotes both the bulk ($K$) and shear ($\mu$) moduli, and $M_1$ and $M_0$ are the Hashin–Shtrikman lower and upper bounds, respectively. The porosity dependence of the shear modulus and dry-state Poisson’s ratio for cemented sands is given by empirical relationships previously proposed for clean.
sandstones (Krief et al. 1990; Arns et al. 2002a),

\[ \mu(\phi) = \mu_{\text{eff}}(1 - \phi)^{m(\phi)} \]  

(31)

and

\[ v_{\text{dry}} = a(\phi) + (1 - (2\phi)^{1/2})v_{\text{eff}}. \]  

(32)

where \( \mu_{\text{eff}} \) and \( v_{\text{eff}} \) are the effective shear modulus and Poisson’s ratio for the mixed mineral constituent. Gassmann’s equations are used to relate the dry and fluid-saturated states.

5.1 Comparison with measured data for clean and shaly sands

Figure 22 shows a comparison between the previously discussed experimentally measured \( V_p \) and \( V_s \) data of Han (1986) and the proposed predictive method (equations (30)–(32)) based solely on a knowledge of the mineralogy. Also shown are the linear least-squares regression fits given by Han (1986) for dry and water-saturated states. The fits for the water-saturated states are given by (11)–(14). Those for the dry states are given by (Han 1986)

\[ V_p(\text{km/s}) = 5.41 - 6.35\phi - 2.87C, \]  

(33)

\[ V_s(\text{km/s}) = 3.57 - 4.57\phi - 1.83C, \]  

(34)

\[ V_p(\text{km/s}) = 5.59 - 6.93\phi. \]  

(35)

\[ V_s(\text{km/s}) = 3.52 - 4.91\phi. \]  

(36)

The proposed predictive method produces estimates for \( V_p \) and \( V_s \) which are of similar quality to Han’s least-squares
Figure 19 Comparison of computed results for the uniform pore-lining model for dry cemented sands with mixed mineralogy with the empirical models given in (20)–(23) (Krief et al. 1990; Nur et al. 1995), where we use $K_{\text{eff}}, \mu_{\text{eff}}$ derived from the simulation (Table 2) in the equations. (a) and (d) show data for quartz/clay and quartz/dolomite systems at a volume ratio of 1:1. (b) and (e) show data for all sand/cement systems considered at ratios of 2:1 and 1:2. (c) and (f) show the systems at ratios of 4:1 and 1:4. (a)–(c) show the predictions of the bulk modulus and (d)–(f) the shear modulus.

Figure 20 Comparison of computed results for model cemented sands with the empirical model of Arns et al. (2002b) given by (24). Agreement is good and much improved on the estimate of most empirical models where $(V_p/V_s)(\phi) = (V_p/V_s)_{\text{mineral}}$.

regression fits. This highlights the potential of the proposed predictive method for producing accurate estimates for velocity/porosity relationships in both clean and shaly sandstones.

5.2 Extensions to three-phase systems

An important advantage of the proposed predictive method is that it is readily extended to multiple mineral phases. The only
Figure 21 Comparison of the results of the simulations for the uniform pore-lining model shaly sands under water-saturated conditions with the equations of Wyllie (dashed line, equation (26)) and Raymer (dotted line, equations (27)–(29)). The mineral ratios are (a) 1:1, (b) 2:1 and (c) 4:1. The Raymer equation gives a better prediction than the Wyllie equation, but in many cases underestimates the value of $V_p$ for a given $\phi$.

The modification required is in evaluating $M_{\text{eff}} = (M_i + M_s)/2$. For multiple mineral phases we use the Hashin–Shtrikman bounds for multiphase systems (Berryman 1995),

$$K_{\text{HS}^+} = \Lambda(\mu_{\text{max}}), \quad K_{\text{HS}^-} = \Lambda(\mu_{\text{min}}), \quad (37)$$

$$\mu_{\text{HS}^+} = \Gamma(\zeta(K_{\text{max}})), \quad \mu_{\text{HS}^-} = \Gamma(\zeta(K_{\text{min}}, \mu_{\text{min}})), \quad (38)$$

where

$$\Lambda(z) = \left(\frac{1}{K(r) + \frac{1}{3}z}\right)^{-1} - \frac{4}{3}, \quad (39)$$

$$\Gamma(z) = \left(\frac{1}{\mu(r) + z}\right)^{-1} - z, \quad (40)$$

$$\zeta(K, \mu) = \frac{\mu}{6} \left(\frac{9K + 8\mu}{K + 2\mu}\right). \quad (41)$$

Since no comprehensive measured multimineral data sets are currently available to test the method, we have computed moduli and velocities for a single three-phase system at a quartz:dolomite:clay ratio of 0.5:0.25:0.25. The computations were made using the grain-overlap model, where spheres of each mineral are placed randomly within the system (no preferential connectivity). The computed data covered a wide range of porosities, $0 < \phi < 0.5$.

Figure 23 shows a comparison between the empirical predictive model (equations (30)–(32)) and the computed data. The prediction for the bulk modulus slightly overestimates the numerical data. The prediction for the shear modulus is excellent despite the fact that the averaged three-phase bounds leads to a $\approx 3\%$ underestimation of $\mu$ for the solid mineral phase. This error is due to the larger variation in bounds with clay, which has a small $\mu = 6.9$ GPa. The dry $V_p/V_s$ ratio is in good agreement with the numerical data displaying a stable fixed point at $V_p/V_s \simeq 1.63$ for all $\phi$. Overall, the agreement is very good for a very complex mineralogy. To the best of our knowledge, no other empirical method currently exists which allows accurate predictions of elastic properties for such a complex mineralogy.

6 SUMMARY

Computer simulations were used to calculate the elastic properties of model cemented consolidated sands composed of two or more mineral phases. Two idealized models for cemented sands were considered: a grain-overlap cement/sand mixture and a pore-lining cement/sand mixture. The mineral phases were clay, quartz and dolomite. Unlike measured data, the computed properties display little noise and allow quantitative comparisons to be made with existing theoretical and empirical models. On the basis of such comparisons we make the following observations and conclusions:

- The effective mineral modulus of the solid mixture shows only small dependence on microstructure. The average of the Hashin–Shtrikman bounds provides a reasonable estimate for the computed modulus data.
- Computed modulus–porosity relationships show little dependence on microstructure. This is consistent with previously proposed models which ignore the distribution of the clay phase. Gassmann’s equations are verified for the porous materials made up of multiple solid constituents.
Figure 22 Comparison of the original data from Han (1986) with the predictive method (equations (30)–(32)) and the linear least-squares fits to the data of Han (1986) (equations (11)–(14) and (33)–(36)). (a), (c), (e), (g) Dry data; (b), (d), (f), (h) wet data. The rows from top to bottom show data for zero clay, clean, intermediate and high clay content.
Numerical computations and experimental data for clay-bearing consolidated sands are in good quantitative agreement.

The bulk modulus–porosity relationships of both Krief et al. (1990) and Nur et al. (1995) fail to describe the numerical data accurately (Fig. 19a). The Krief equation (31) does however provide a very good match for the shear modulus data (Fig. 19d–f). An accurate empirical $v-\phi$ or $V_p/V_s-\phi$ relationship (equation (32)) for dry sands also matches the numerical data very well (Fig. 20).

The Raymer equation (29) is the best modulus–porosity model for water-saturated conditions, but it consistently underestimates the computed $V_p-\phi$ data. The Wyllie equation provides an unsatisfactory estimate of the computed $V_p-\phi$ data.

A new empirical model for cemented multimineral consolidated sandstones is proposed. The model uses the empirical Krief equation for the shear modulus (equation (31)) and the empirical equation of Arns et al. (2002a) for the Poisson’s ratio of a dry sand (equation (30)). The effective mineral moduli are determined from the average Hashin–Shtrikman bounds. Gassmann’s equations are used to predict the fluid-saturated states. The model predicts the measured data of Han (1986) with a similar degree of accuracy to a linear least-squares fit.

The new empirical model is extended to three or more mineral phases. Comparison with model three-phase mineralogy data is encouraging.

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