A rock physics model for analysis of anisotropic parameters in a shale reservoir in Southwest China
A rock physics model for analysis of anisotropic parameters in a shale reservoir in Southwest China

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Abstract
A rock physics model is a very effective tool to describe the anisotropy and mechanical properties of rock from a seismology perspective. Compared to a conventional reservoir, modelling a shale reservoir requires us to face two main challenges in modelling: the existence of organic matter and strong anisotropy. We construct an anisotropic rock physics workflow for a typical shale reservoir in Southwest China, in which the organic matter is treated separately from other minerals by using a combination of anisotropic self-consistent approximation and the differential effective medium method. The standard deviation of the distribution function is used to model the degree of lamination of clay and kerogen. A double scan workflow is introduced to invert the probability of pore aspect ratio and lamination simultaneously, which can give us a better understanding of the shale formation. The anisotropic properties of target formation have been analysed based on the proposed model. Inverted Thomsen parameters, especially the sign of delta, are analysed in terms of the physical properties of rock physics modelling.

Keywords: shale rock physics, anisotropy, inclusion theories, pore aspect ratio, clay lamination

(Some figures may appear in colour only in the online journal)

Introduction
Shale-related studies have recently increased rapidly due to more unconventional resources being explored in shale sequences. Shale has been proven to show the property of transverse isotropy (TI) and there are multiple causes of shale anisotropy. Ignoring shale anisotropy can induce significant errors in geophysical processing and interpretation (Sayers 2013).

The rock physics model is a very effective tool used for linking the anisotropy and mechanical properties of rock to the geophysical data (Spikes et al. 2007, Mavko et al. 2009). Many models and empirical relationships have been constructed for conventional sand reservoirs, while the rock physics models for unconventional shale reservoirs are still controversial, due to anisotropic shale reservoirs being much more complicated than isotropic sand reservoirs (the anisotropy of a sand reservoir is negligibly small). Many experts have tried to construct a proper shale model and not found it to be easy due to the complicated intrinsic properties of shale. These properties contribute to the anisotropy of shale. Hence, describing the anisotropy of shale is the key to the construction of a shale model (Mavko et al. 2009).

Many factors can contribute to the anisotropy of shale. Based on published research, the causes of shale anisotropy can be summarized within three main aspects. (1) A preferred orientation of clay and kerogen particles can be used to explain...
the VTI quality properly (Vernik and Nur 1992, Vernik and Liu 1997, Arne Johansen et al 2004); (2) SEM (scanning electron microscopy) and XRD (x-ray diffraction) observations shows that a flat pore shape and some micro-fractures exist in shale, which further enhances the TI properties of shale (Sayers 1994); (3) The clay mineral has its own intrinsic anisotropy (Sayers 1994, 2005, Sondergeld et al 2010, Guo et al 2014). In our study, we intend to construct a rock physics model of shale which can take different causes of shale anisotropy into consideration.

Organic matter and the clay mineral largely contribute to the shale anisotropy. Many experts have found that the vertical transverse isotropy (VTI) property of shale comes from the partial alignment of clay and laminated kerogen (Vernik and Nur 1992, Sondergeld et al 2010, Sayers 2013). On the one hand, kerogen, as representative organic matter, has very unique physical qualities, such as extremely low density and velocity compared with other minerals. In addition, the bulk modulus and shear modulus of kerogen is as low as 2.9 GPa and 2.7 GPa compared with those of quartz (37 GPa and 44 GPa, respectively) (Mavko et al 2009), which means organic matter is, in a sense, more like a fluid than a mineral, even though it has a solid phase. So kerogen may exist either in the matrix or in pores, which may influence the anisotropy of shale. In addition, organic matter is the origin of the shale reservoir, and can transfer to hydrocarbons under certain situations. Many irregular pores will appear during the transformation, which also contributes to the shale anisotropy. On the other hand, the lamination of clay is also significant, since the volume fraction of clay is relatively high in shale and the kerogen and clay are usually embedded within each other, which is the main contribution to the anisotropy of shale. So how to model the kerogen and clay in shale is an important question in model construction.

In order to model the effect of kerogen and clay in shale, different methods have been proposed with a certain emphasis. In order to focus on the lamination of clay and kerogen, the Backus average is commonly used (Backus 1962, Vernik and Nur 1992, Vernik and Landis 1996, Guo et al 2012). Vernik et al (1992) treat organic rich shale as a 1D layered medium consisting of layers of shale and kerogen using the Backus average (Sayers 2013). The predicted C_{33} does not fit the real data well, so they introduce a parameter to correct the deviation (Vernik and Landis 1996). Guo et al (2013) pointed out that the Backus average works well only when the shale has a relatively simple mineralogical composition. Hence, the Backus average is not sufficient to model kerogen in shale. Recently, the differential effective medium (DEM) method has been used to model the kerogen in shale (Bandyopadhyay 2009, Wu et al 2012). The DEM method can be used to treat different compositions as inclusions and can control the anisotropy of the rock by changing the aspect ratio of each inclusion, which is useful for modelling the pore shape and microstructure of shale. However, the DEM method has a vital drawback in that you need to set a background material and add the other inclusions step by step. Different orders of the additions can cause different predictions. Hence, many experts have tried to find the best workflow for shale modelling. Bandyopadhyay (2009) and Wu (2012) claimed that Vernik’s data can be modelled well by using the anisotropic DEM theory with kerogen as the background and adding the other minerals into the kerogen. However, many experts found that the scanning electron microscope (SEM) images of organic-rich shale show patches of kerogen occupying discrete spaces within the in-organic rich matrix of shale (Sondergeld et al 2010, Curtis et al 2012). So a disagreement arises, and Sayers (2013) claimed the disagreement may result from disconnectivity between clay and kerogen.

Zhu et al (2012) have proven that kerogen can be modelled in a ‘fluid way’. They add kerogen into shale by using a solid substitution equation proposed by Ciz and Shapiro (2007). This solid substitution function was first used to model the heavy oil in pores, and Zhu et al (2012) have applied it to organic shale modelling since both kerogen and heavy oil have a non-zero shear modulus.

Hornby et al (1994) were the first to combine the specific catchment area (SCA) and DEM methods to model the clay-water mixture. However, kerogen is not taken into consideration in Hornby’s study. In this study, we treat kerogen in a ‘fluid way’, and employ the SCA + DEM method to model the biconnected clay–kerogen mixture and try to solve the disagreement described by Sayers (2013). As mentioned above, the kerogen is more like a fluid than a solid. And the connectivity between clay and kerogen is more significant than clay and pores, since the porosity of shale is usually extremely low and isolated, while the connectivity between clay and kerogen is more obvious in SEM images (Sondergeld et al 2010, Curtis 2012). The kerogen and clay often intermingle with each other, and form the background of shale with patchily occupied quartz (Hornby et al 1994).

In addition, clay lamination is another significant origin of shale anisotropy. In Hornby’s paper (1994), the authors modelled the effect of clay lamination by using a normal distribution function (named D(n) in his paper). Xu et al (2010) combine the probability density function with the DEM method to model the preferred orientation of different pores. In this paper, we manage to evaluate the effect of the standard deviation by parametrizing it as clay lamination (CL) and try to link it with the anisotropy of shale.

The normal distribution function is controlled by two parameters: the mean value and the standard deviation. The mean value represents the bedding angle, while the standard deviation could represent the extent of lamination. A mean value of the distribution function could be derived from the good quality SEM images of core samples in Hornby’s paper, but the standard deviation information is not always be available. In this sense, if we parameterize the standard deviation, and set the mean value to a constant or zero, we can model the properties of clay lamination.

Hence, the motivation for modelling clay lamination using standard deviation can be summarized into two parts: Firstly, we intend to model the anisotropy of shale with limited data, because analysis of standard deviation can provide us with information that is difficult to derive. Secondly, we assume that setting a mean value equal to small constants or zero with a statistically varied standard deviation may be more general.
than setting standard deviation as a constant, since the extent of lamination cannot be the same for formations of different depths.

Based on our anisotropic rock physics model for organic shales, we test the validity of our model by estimating the elastic properties of a real data set from southwest China. By using a double scan workflow, we can invert the anisotropic parameters from $V_p$ and $V_s$ well logging data; Thomsen parameters, especially the sign of delta, are discussed in terms of pore aspect ratio, clay lamination and mineralogy.

Inclusion theories

Inclusion theory is one of the typical effective medium theories used to estimate the elastic properties of realistic rock. The rock is usually assumed to be a homogeneous solid which has the equivalent properties of a heterogeneous solid with a complicated microstructure (Das and Batzle 2009).

The SCA and DEM are all inclusion theories (equations for each theory are shown in the appendix A). As the name implies, inclusion theories treat all the components of rocks as inclusions, and they also introduce an important parameter: the aspect ratio to control the shape of individual inclusion, which can help us to control the pore shape and microstructure. It is widely acknowledged that the pore geometry of shale is very complicated and different types of mineral may exist in shale (Sondergeld et al 2010, Guo et al 2012), which make inclusion theories a popular option for shale modelling (Bandyopadhyay 2009, Wu et al 2012, Jiang and Spikes 2013, Guo et al 2014).

As mentioned above, how to model the organic matter in shale is the key to the construction of a shale model. Many experts have paid attention to both the SCA and DEM methods in recent years. But at this stage, the issue of choosing the best method for organic modelling is still under discussion, since both the SCA and the DEM method have their limitations.

In this section, we show the limitations of the SCA and DEM methods and try to test the feasibility of using the SCA + DEM method to model kerogen in shale, which can help to solve the disagreement described by Sayers (2013), as mentioned above.

Differential effective medium (DEM)

The DEM method performs well in some shale rock models (Bandyopadhyay 2009, Wu et al 2012). Its main drawback is the order problem. Before applying the DEM method, we need to choose one mineral as the background mineral and add the other minerals into the background. If we choose a different background mineral, we can get different results, even if we keep the other parameters unchanged. This kind of theoretical error is hard to eliminate. The figures below show different results obtained by changing the background material.

Figure 1 illustrates the DEM modelling results. Red lines represent the predicted results using anisotropic DEM with clay as background, and blue lines are the predicted results with kerogen as background. As marked in the figures, the solid and dashed lines indicate the scenarios of aspect ratio of inclusion equal to 0.1 and 1, respectively. As shown in figure 1, different background gives different result while using anisotropic DEM, and this difference decreases as aspect ratio increases. The prediction of $C_{44}$, $C_{66}$ are similar to $C_{11}$ and $C_{33}$, so we just show two figures here.

Combination of the SCA and DEM methods

Although the DEM method has an order problem, it can help the SCA method solve the bi-connected problem. The anisotropic SCA + DEM method combines the advantages and gets rid of the individual disadvantages of both the SCA and DEM methods. Firstly, SCA is performed to build a biconnected effective medium with equal concentration. Then, the effective medium is adjusted to the desired concentration by using the DEM method. The advantage of the DEM method is that it can preserve the connectivity of any phase which is connected (Hornby et al 1994). So, in the first step, 50% concentration is in the connected range of the SCA method and the DEM method can extend the connectivity range to the whole
percentage range. Figure 2 indicates the biconnected range for the clay–kerogen mixture. Meanwhile, the anisotropic SCA + DEM method does not need the background phase to be set, which avoids the disadvantage of the DEM method.

Validation of the template

In order to test the feasibility of building a clay–kerogen block using the SCA + DEM method rather than other theories, we use several theories which have been proposed to build theoretical relationships between kerogen concentration and the elastic properties of organic-rich shale, for example, traditional Backus average and anisotropic DEM theory. These theories are compared with the rock physics model introduced in this paper, and the measured data presented in Vernik and Landis (1996) are used as a reference. The properties of kerogen and shale are shown below quoted from Sayers (2013) who calculated the elastic constant based on the measured velocities given by Vernik and Landis (1996).

Four types of theoretical theories are modelled with varying aspect ratio in figure 3: (a) the solid red lines indicate the result of using the traditional Backus average; (b) the solid magenta lines indicate the scenario of adding kerogen inclusion into the shale background using anisotropic DEM; (c) the solid blue lines indicate the scenario of adding shale into kerogen background using anisotropic DEM; (d) the dashed green lines indicate the scenario of combining shale and kerogen as a bi-connected mixture by using the anisotropic SCA + DEM method. The black dots are real data points from Bakken shale given by Vernik and Liu (1997). As shown in figure 3, the marked numbers indicate the corresponding pore aspect ratio. According to the analysis of Sayers (2013), the modelled results of Backus average indicate the scenario of aspect ratio = 0. All the elastic stiffness coefficient and Thomsen parameters are shown here.

Comparing the modelling results with real data dots measured by Vernik and Liu (1997), in agreement to the analysis results of Vernik et al (1997) and Sayers (2013), the traditional Backus average performs well only in prediction of vertical elastic velocities ($C_{11}$ and $C_{66}$) related to vertical P and S wave velocities. The inclusion theories can get better results for both vertical and horizontal elastic velocities by varying the aspect ratio of inclusion.

For horizontal velocities, indicated by $C_{11}$ and $C_{66}$, the solid magenta lines show that the case of kerogen inclusion in shale is better than the Backus average, but it is still an overestimate. The blue and green lines coincide well with the data, which testifies that the SCA + DEM method, like the DEM with kerogen background, has the ability to model kerogen in shale.

The effects of clay and kerogen lamination

After constructing a biconnected clay–kerogen mixture, we try to model the lamination property of shale. In a real shale reservoir, the major portion of clay is laminated, while a small portion of it is distributed randomly (Hornby et al 1994). So we rotated and combined many identical clay–kerogen blocks by using the Bond transform and Voigt–Reuss–Hill (VRH) average (related equations are shown in the appendix A). The rotated angle for each block is satisfied with a normal distribution function. The mean value of the normal distribution is fixed at zero since the majority of blocks remain flat, while the standard deviation (we use CL to represent it in the following article) varies in order to model the degree of the lamination. When CL equals one, all the clay–kerogen blocks stay flat which gives a strong VTI property. As CL increases, the VTI property decreases, meaning that more and more blocks are rotated. Figure 4 illustrates the probability density with CL equal to 30, 60 and 90. The curves are symmetric relative to 0 degrees which means the mean value equals zero, and as CL increases, the probability density of zero degree decreases, which means more and more blocks are flat. Hence, CL can control the degree of lamination and thus control the anisotropy of shale.

In order to test the feasibility of using the Bond transform and VRH average to model the lamination of shale, we vary the standard deviation to examine the variation of predictions.
Figure 3. The prediction elastic constants and Thomsen parameters versus kerogen concentration, calculated from measured velocities from Vernik and Liu (1997) in Bakken shale based on different theories. And the anisotropic SCA + DEM theory gives the best prediction.
Figure 5 shows how the standard deviation can control the lamination and influence the anisotropy of clay. The elastic properties for figures 5(a) and (b) are quoted from Sayers (2013): \( C_{11} = 85.6 \text{ GPa}, C_{33} = 65.5 \text{ GPa}, C_{44} = 24.6 \text{ GPa}, C_{66} = 29.7 \text{ GPa} \) and \( C_{13} = 21.1 \text{ GPa} \).

Figures 5(a) and (b) show the variation of the stiffness tensor with standard deviation. We find the anisotropy of the mixture reduces as the standard deviation increases.

In order to analyze the sign of delta with respect to CL, we quoted two shale samples from Wang (2002); one sample has a positive delta value and the other has a negative one. Then we treat them as a shale block, after rotating and combining many identical blocks according to CL, the corresponding Thomsen parameters illustrate how CL influences anisotropic parameters.

The elastic properties for figures 5(c)–(e) are quoted below: For sample 1 \( \varepsilon = 0.317, \gamma = 0.513 \) and \( \delta = -0.054 \). And for sample 2, \( \varepsilon = 0.121, \gamma = 0.138 \) and \( \delta = 0.046 \).

As the CL value increases, both \( \varepsilon \) and \( \gamma \) decrease. The most significant pattern is that no matter the initial sign of \( \delta \) value, it always varies towards to a very small positive value, which is similar to the modelling analysis of Sayers (2005) and is discussed in detail in figures 15(d)–(f).

**Shale rock physics model**

The key factors in our model are that: firstly, the anisotropic SCA + DEM method is performed to model the biconnected kerogen–clay mixture. Since the elastic property of kerogen is more like clay than other minerals, the clay–kerogen block is constructed using the SCA + DEM method. Secondly, the blocks are rotated and combined in order to model the preferred orientation of clay and kerogen. Since Arne Johansen et al (2004) noted that the effect of several statistical orientation distributions results in a slight difference for the purpose of VTI modeling, we set the angles of the blocks to satisfy a normal distribution with mean value equal to zero according to the VTI property of shale (Sondergeld 2010). The orthotic properties of shale can be modelled by adding vertical fractures into the VTI background.

The workflow of our organic shale model is shown in figure 6.

1. Isotropic kerogen and isotropic clay are mixed to build a biconnected clay–kerogen block by using the anisotropic SCA + DEM method.
2. Many identical blocks are rotated to different angles which are normally distributed. Bond transform is used to calculate the elastic stiffness of all rotated blocks, and the VRH average is used to combine all these rotated blocks to form the preferred orientated clay–kerogen background.
3. Then, the VRH average is used to calculate the elastic stiffness of other brittle minerals present in the rock.
4. Finally, considering the preferentially orientated clay–kerogen mixture as the background, we use the anisotropic DEM to add an isotropic brittle mixture and pores into the background successively to form the final effective mixture.

There are three steps in which the DEM is used, which are:

(a) To add brittle minerals, like quartz, calcite, etc, into the clay–kerogen background.
(b) To add clay–kerogen-related pores into the clay–kerogen block.
(c) To add sand-related pores into the whole mineral background to build a dry frame.

In order to choose the best workflow for our target formation, we take geological information into consideration. Based on the geological report of the target formation, it is marine shale with high diagenesis and high maturity level properties. The high diagenesis effect illustrates the good lamination of target area. A logging cut report also shows that the clay and kerogen often couple with each other. Hence we assume clay and kerogen are inter-coupled and form the laminated background with isotropic brittle minerals developed in it.

Hence, for step (a), clay and kerogen are firstly modelled without the brittle minerals. The reason why we choose SCA + DEM instead of SCA or DEM is that the volume concentration of clay and kerogen varies for the whole depth, and it is hard to choose either clay or kerogen as the background material here. Meanwhile, the concentration of kerogen may exceed the biconnected range of the SCA. So we choose symmetric SCA + DEM to model the clay and kerogen mixture and try to keep the connectivity of clay and kerogen. Then the lamination is modelled by using the normal distribution function.

After the clay–kerogen background is formed, the remaining brittle mixture is added into it by using anisotropic DEM. Because the inclusion phase of DEM is usually on isolated existence in a background material due to the high frequency assumption, and the patch developed isotropic brittle minerals are usually isolated in a clay–kerogen background, we choose anisotropic DEM to add isotropic brittle minerals into the anisotropic clay background, as discussed in Bandyopadhyay (2009) and Wu (2012).

The porosity effect is considered in both step (b) and step (c). The geological report shows that clay-related inter-particle
pores, organic-related pores and micro-fractures are the main pore type in the target zone. Because micro-fractures are mostly filled by cementation in our formation, clay- and organic-related pores are the main pore type we need to consider. We follow the work of Xu et al. (2010) to handle the porosity. The reason for using DEM in step (b) is that we assume clay–kerogen-related pores are isolated, which again satisfies the high frequency assumption of DEM. For step (c), the sand-related pores are assumed to be connected and it can be modelled by adding dry pores into the mineral background and substitute fluid content by using the Brown–Korring method. A detailed discussion can be found in Xu et al.’s work (2010).

Three types of pores are considered in Xu et al.’s work. The total pore space is divided into three parts: clay-related pores, sand-related pores and micro-cracks. The volume of clay-related and sand-related pores can be estimated using normalized shale volume, and the porosity of cracks can be estimated based on an empirical relation between overburden stress and crack porosity (see the appendix A).
All the pore types are added to the mineral background simultaneously based on the method proposed by Xu et al. (2010). Xu’s method adds a small portion of all pore types proportionally at each iteration, which avoid the asymmetry problem resulting from the order problem of DEM. Although we do not discuss the pore orientation, we do consider the orientation of clay–kerogen block.

**A case study from the Sichuan basin, southwest China**

Figure 7 illustrates real well-logging data from well A. The target formations are the lower part of the Longmaxi shale formation and Wufeng shale formation at depths between 2045 and 2065 m. Gamma ray, porosity, P and S wave velocity, total organic carbon, density, \( V_p/V_s \) ratio and Poisson’s ratio are plotted from left to right. Two gamma ray curves are shown in the left-most column. The red curve indicates total gamma value and the blue one shows the gamma value without uranium. The majority of the radioactive element of kerogen comes from uranium. The gap between these two curves can help us to locate our target zone, and the larger gap presents the higher TOC fraction existing in the corresponding formation. The other logging curves also show typical features of a shale reservoir: relatively high porosity compared with the surrounding formations, low P and S wave velocities and low density caused by the presence of clay and kerogen minerals, and a high total organic carbon (TOC) value. The ternary shows the mineralogy of the target depths. The dot colour indicates the TOC value, from which we can find that a lower TOC corresponds to lower clay content. The TOC value is calculated based on CRA procedure and calibrated by using core data.

In terms of porosity, since we have very limited data. There is only one porosity curve available which is total porosity, and it is inverted by using the traditional CRA procedure. Based on the logging interpretation report, the porosity and the volume fraction of mineral are calculated by the crossplot of the compensated neutron curve and the compensated density curve.

The porosity of the target formation is below 5% and that of surrounding formation is even lower. Since the geological time of our target formation is Upper Ordovician, which is very old, the formation is fully compacted and the primary porosity space is nearly closed.

Meanwhile, the TOC value increases as the porosity increases, which gives a straightforward idea the porosity is related to TOC. The analysis of cores and cuttings shows the formation is marine face formation and the maturity of TOC is high with a Ro value equal to 2–2.5. Some micro-pores and micro-cracks can be found in cores which may have been generated during thermal evolution.

By combining the geological background and TOC analysis of the target zone, we believe that the porosity is mainly contributed by TOC related pores. Since the \( V_m \) decreases as porosity increases in the target area, we think it may not be proper to divide the pore space into clay-related pores and quartz-related pores based on \( V_m \) for our formation. In addition, since the porosity is really low (<5%), the divided porosity may be even lower, which may cause numerical error during forward modelling.

So we simplify our model and add the total porosity into mineral background by using the DEM theory. The reason why we use DEM is that the majority of pores are clay–kerogen related pores and the porosity is very low, which satisfies the high frequency assumption of DEM and we assume all the pores are isolated. (We use the same method to deal with clay-related pores, just like Xu et al. (2010)).

**Microstructure inversion and S wave prediction**

In this section, we model and analyze the pore geometry of the target zone based on our model. Both anisotropic SCA and DEM theories are used in our model. The SCA and DEM are all inclusion theories (Hornby et al. 1994). As mentioned earlier, pore aspect ratio is the key parameter in inclusion theory. Pore aspect ratio can be used to model the un-spherical pore shapes in shale, which is one of the main origins of shale anisotropy. Although the pore aspect ratio is so significant, it is hard to measure directly.
A 3D template method is proposed to invert for the pore aspect ratio. 2D rock physics templates are usually applied to illustrate the relationship between pore aspect ratio and other elastic parameters (such as velocity or impedance) and further inversion (Xu and Payne 2009, Jiang and Spike 2013). This procedure needs to appropriately estimate the volume fractions of each mineral, which remains unchanged. So the common way to invert for pore aspect ratio is to apply an average volume fraction of each mineral for the target depths to build the template, and then invert for the pore aspect ratio by using the template. However, the minerals’ volume fractions in shale could have a huge variation from sample to sample. The new template includes the volume fraction of clay and kerogen. In the application to real log data, it is difficult to analyze...

Figure 7. (a) Well logging data from south China. Panels from left to right indicate GR, porosity, $V_p$, $V_s$, TOC, Density, $V_p/V_s$ and Poisson’s ratio. The target area is overlaid in yellow colour (b) Ternary of mineralogy of target depths colour-coded by TOC values. (c) Mineralogy of target depths shows the volumetric fractions of constituents.

Table 1. The properties of Kerogen and Shale quoted from Sayers (2013).

<table>
<thead>
<tr>
<th>Component</th>
<th>Density (g cm$^{-3}$)</th>
<th>$C_{11}$ (GPa)</th>
<th>$C_{13}$ (GPa)</th>
<th>$C_{44}$ (GPa)</th>
<th>$C_{56}$ (GPa)</th>
<th>$C_{12}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kerogen</td>
<td>1.25</td>
<td>9.8</td>
<td>9.8</td>
<td>3.2</td>
<td>3.2</td>
<td>3.4</td>
</tr>
<tr>
<td>Shale</td>
<td>2.73</td>
<td>85.6</td>
<td>65.5</td>
<td>24.6</td>
<td>29.7</td>
<td>21.1</td>
</tr>
</tbody>
</table>
every volume fraction of the minerals because the mineral constitution of shale is complicated. So the volume fraction of ductile minerals (combination of clay and kerogen which represented by $V_{sh}$) is used to represent the mineralogy of the rock. The material properties are shown in table 2, quoted from Mavko (2009).

Figure 8 shows the 3D template: the x-axis, y-axis and z-axis represent the volume fraction of ductile minerals ($V_{sh}$), porosity and elastic wave velocity, respectively. The top and bottom coloured curve represents the modelling elastic wave velocity for pore aspect ratio equal to 1 and 0.01 respectively. The template needs to be adjusted for real data set. The aspect ratio of brittle minerals can be treated as a fitting parameter which can make all the data points be covered by the top and bottom curve, which means all the data points can be modelled by our model with pore aspect ratio changing from 0.01 to 1. Here, we set it to be 0.8 for our data set.

A similar procedure is performed on both P and S wave data. The pore aspect ratio seems more sensitive to the S wave. Besides, these two curves only coincide with each other when porosity equals zero, which means that the pore aspect ratio cannot influence the modelling results when porosity equals zero.

By using the 3D aspect ratio template, we can invert for the pore aspect ratio. The P wave velocity is set as the object parameter, and then many modelling P wave velocities are modelled by varying the pore aspect ratio. The value of aspect ratio which minimizes the difference between the modelling P wave velocity and real P wave velocity is the inverted result. The corresponding object function is shown as below for P wave templates:

$$\left| V_p - V_{p\_model} \right| \rightarrow \text{min}.$$  (1)

The pore aspect ratio, S wave velocity and Thomsen anisotropic parameters have been predicted by using the P wave template. In figure 9(a), the left two panels show the predicted $V_p$ and $V_s$ respectively. The red lines represent the modelled result and the blue lines illustrate the real measured velocity. The predicted results coincide with the measured data well in the majority of the depth range, which proves the feasibility of our model.

In addition, S wave data is also available. The same procedure is performed on S wave data to further test our model.

### Table 2. Material properties (Carcione 2000, Mavko 2009, Guo 2014).

<table>
<thead>
<tr>
<th>Material</th>
<th>Quartz</th>
<th>Clay</th>
<th>Calcite</th>
<th>Dolomite</th>
<th>Kerogen</th>
<th>Fluid (brine)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$ (GPa)</td>
<td>37</td>
<td>25</td>
<td>77</td>
<td>95</td>
<td>2.9</td>
<td>2.2</td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>44</td>
<td>9</td>
<td>32</td>
<td>45</td>
<td>2.7</td>
<td>0</td>
</tr>
<tr>
<td>Density (kg m$^{-3}$)</td>
<td>2650</td>
<td>2550</td>
<td>2710</td>
<td>2870</td>
<td>1300</td>
<td>1040</td>
</tr>
</tbody>
</table>
The S wave velocity is set as the objective parameter instead of P wave velocity and the other parameters are kept unchanged. The object function is shown in equation (2).

$$|V_i - V_{i\_model}| \rightarrow \text{min}.$$  

(2)

By using 3D templates in figure 8, the predicted P and S wave velocities can be obtained, which are shown in figures 10 and 11, and they match well with measured data. The predicted P wave result seems more solid than the predicted S wave, which may be because the S wave is more sensitive to pore aspect ratio, as shown in figure 9(b).

Besides, the error may also be caused by the fixed standard deviation of the normal distribution function used to model the lamination of clay and kerogen. The effect of lamination is not considered properly in this inversion procedure. For this data set, we set the CL equal to 20 while inverting for the pore aspect ratio, since it can help to construct a good 3D template which can match the data points well. In the next section, we will try to eliminate this difference by taking lamination into consideration.

**Effect of lamination of clay and kerogen**

If we select the first panel in figure 10 and the second panel in figure 11 together with the clay volume fraction, we are able to find some common laws. For both the P wave and S wave, as SH increases, the error between the predicted result and the real velocity increases in the majority of depth ranges (as shown in the shaded areas). So does the different extent of lamination of clay and kerogen cause the mis-prediction?

The left two panels are the predicted P and S velocity by setting S and P velocity as the fitting parameter, respectively. The inversion procedure sets the pore aspect ratio as the only variable which can influence the prediction. Another key factor in our model, the standard deviation, equals 20 for the whole depth range. However, the laminated situation for clay and kerogen cannot be the same for the whole range. Hence, we need to take the lamination effect into consideration during inversion.

The workflow for CL estimation is shown in figure 12. We input both P and S wave velocity to our model, and invert for clay and kerogen lamination by using a double scan procedure.

In this workflow, we set CL as a parameter to represent the value of standard deviation, and Asp indicates pore aspect ratio. Repeating the work in the last section, we input well logging data, such as mineralogy, density, P wave and S wave velocity into our model. Then we can build up a 3D template for pore aspect ratio inversion. If we set $|V_p - V_{p\_model}| \rightarrow \text{min}$ as the object function, the error between predicted $V_p$ and real $V_p$ is defined as $\Delta V_p$, and the best fitting pore aspect ratio is Asp_p. If we use $V_s$ as an object parameter, and repeat the same procedure, $\Delta V_p$ and Asp_s can also be obtained.

For each depth, we compare two predicted errors: $\Delta V_p$ and $\Delta V_s$. The predicted pore aspect ratio which accompanies the minor error is selected to be Asp_fix. Then the effect of lamination is taken into consideration; we set the standard deviation value—CL uniformly distributed from 0 to 90 with increments equal to 5, and the pore aspect ratio also varies uniformly from Asp_fix-0.03 to Asp_fix+0.03 with increments equal to 0.002. Hence 31 aspect ratios and 19 CLs values are calculated based on our model for each depth. And if the predicted P and S wave velocities ($V_p\_model$ and $V_s\_model$) satisfy the final object equation shown in equation (3), the corresponding pore aspect ratio and CL value will be accepted.

$$\sqrt{(V_p\_real - V_p\_model)^2 + (V_s\_real - V_s\_model)^2} \rightarrow \text{min}.$$  

(3)

In addition, the probability of occurrence for every possible pore aspect ratio and CL can be obtained for each depth.
Finally, the best results can be found with the highest probability for both pore aspect ratio and CL.

Figure 13 illustrates the probability for both CL and pore aspect ratio for depth = 2058 m. The x and y axis illustrate the uniformly distributed CL and pore aspect ratio. The initial input data is CL = 20 and Asp = Asp_fix, which is shown as a black star. After the double scan workflow, the best result shifts to values of CL = 1 and Asp = Asp_fix-0.004 (shown as a golden star). Repeating the procedure for all depths, the final prediction is shown in figure 14. From the left two panels we can clearly find that the predicted results are much better than previously, and the pore aspect ratio and clay–kerogen lamination can be obtained simultaneously as well.

The final anisotropic prediction shows that the formation has strong anisotropy. The range for ε and γ is between 0.1 and 0.4 and δ has both positive and negative values with a minimum value of around −0.05.

In order to link anisotropic properties with rock physics parameters, we draw several crossplots (figure 15) between...
each Thomsen parameter and colour-coded them by values of pore aspect ratio, CL, porosity, and volume concentration of clay and kerogen respectively.

The data points in figures 15(a)–(c) are colour-coded by inverted clay lamination value (labelled CL). The relationship seems not as clear as effective crack density, the value seems not as clear as for asp. Sayers (2005) argues that the relationship between CL and pore aspect ratio is the premise of CL inversion. Hence, CL is primary effect factor and CL is secondary. So the accuracy of CL inversion procedure, we only consider that CL varies from 1 to 100. Figure 13 illustrates the predicted probability; the probability range of the pore aspect ratio is narrow comparing with CL, which illustrates that the pore aspect ratio is the primary effect factor and CL is secondary. So the accuracy of pore aspect ratio is the premise of CL inversion. Hence, CL is opposite to pore aspect ratio. High crack density corresponds to high $\epsilon$ and $\gamma$. Meanwhile, crack density is sensitive to $\delta$, and $\delta$ decreases as effective crack density increases.

For figures 3(g)–(i), in order to consider pore aspect ratio and porosity effect simultaneously, we colour-coded data points by using effective crack density (defined by $3c/4\pi\alpha$). The reason we named it ‘effective crack density’ is that, for this dataset, we simplify our model and use only one effective pore aspect ratio to model the whole pore space. The porosity we use here is also total porosity. Hence, the colour-coded value seems a little large. The effective crack density seems to high $\epsilon$ and $\gamma$. Meanwhile, crack density is sensitive to $\delta$, and $\delta$ decreases as effective crack density increases.

The reason we named it ‘effective crack density’ is that, for this dataset, we simplify our model and use only one effective pore aspect ratio to model the whole pore space. The porosity we use here is also total porosity. Hence, the colour-coded value seems a little large. The effective crack density seems to high $\epsilon$ and $\gamma$. Meanwhile, crack density is sensitive to $\delta$, and $\delta$ decreases as effective crack density increases.

Figures 3(j)–(l) indicate the relationship between anisotropic parameters and mineralogy. The background colour indicates the volume fraction of clay and kerogen. A dark colour indicates high concentration of brittle minerals. Even not as clear as effective crack density, the $\delta$ value is correlated to mineralogy to some extent. The majority of light colour points show a negative $\delta$ value, which means the existence of clay and kerogen can result in a negative $\delta$ value.

Two main parameters can control the accuracy of prediction of anisotropic parameters during rock physics modelling. One is the aspect ratio of inclusion while using SCA + DEM, and the other one is CL. Figures 3(e)–(g) and 5(c)–(e) illustrate how the anisotropic parameters vary according to them.

The pattern for epsilon and delta seems easier than that for delta. In terms of aspect ratio (AP), low value of AP can result in high values of epsilon and gamma, and as the volume fraction increase up to nearly 50%, the epsilon and gamma reach their peak points. Comparing with figures 15(b) and (c), high epsilon and gamma always correspond to low AP. As mentioned above, setting a minimum boundary for AP during AP inversion (for example AP is always greater than 0.01) is quite important and can help us to avoid unstable results. Meanwhile, besides AP, the volume concentration of inclusion can also influence anisotropic predictions. The unstable volume range for epsilon and gamma is around 40–60% and that for gamma is around 30%, which means that the prediction error may increase while the volume concentration of inclusion is near the unstable range.

In terms of CL, both epsilon and gamma decrease as CL increases according to figures 5(c) and (d). As CL increases, it becomes less sensitive to anisotropic parameters, so in the CL inversion procedure, we only consider that CL varies from 1 to 100. Figure 13 illustrates the predicted probability; the probability range of the pore aspect ratio is narrow comparing with CL, which illustrates that the pore aspect ratio is the primary effect factor and CL is secondary. So the accuracy of pore aspect ratio is the premise of CL inversion. Hence, CL is
more like a compensation or ‘regulator’ for anisotropic parameters. In terms of figures 15 (d)–(f), high epsilon and gamma always result from low CL, since high lamination gives high anisotropy. However, low epsilon and gamma cannot equal a high CL, since it may result from a low aspect ratio of inclusion. On the country, a high CL value always corresponds to low epsilon and gamma, which illustrates the scenario of poor lamination with low anisotropy.

Discussion and conclusion

In this paper, we choose an appropriate rock physics workflow for a typical shale reservoir from southwest China. Different origins of anisotropy of shale are considered in our workflow. The kerogen in shale is simulated using anisotropic SCA + DEM theory which can help to build a biconnected clay–kerogen mixture. The degree of lamination of clay and
kerogen is modelled by introducing the standard deviation of the distribution function.

For data analysis, a 3D template is constructed based on our model. The mineralogy effect is taken into consideration, which makes the model more realistic than the usual methods. Reservoir properties, such as pore aspect ratio, which indicates the microstructure of reservoir and S wave velocity, have been predicted using the 3D template. The predicted results coincide well with the measured data. In addition, if S wave velocity is available, we introduce a double-scan workflow to invert for the probable pore aspect ratio and CL which give us a better understanding of the anisotropic properties of underground shale formation.

Since both positive and negative $\delta$ values occur in our target area, Thomsen parameters are discussed in terms of pore aspect ratio, clay lamination and mineralogy. Our results indicate the sign of $\delta$ are related both to pore aspect ratio and the lamination of clay and kerogen. Both high effective crack density and well laminated clay can contribute to the negative sign of $\delta$. In addition, the patterns between anisotropic parameters and rock physics parameters and the potential deviation during prediction have been discussed.

Nevertheless, we have to admit that the rock model has only been tested in our target area. The other in situ shale reservoir is much more complicated than we thought. The uncertainties in our modelling may be caused by the assumption of theoretical models. In addition, the pore fluid in shale may be influenced by the maturity stage of the organic matter. Hence, how to handle the pore fluid in shale is a problem that has yet to be solved. Finally, all material properties may vary for different reservoirs. How to obtain accurate properties is also significant.

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Appendix A

Anisotropic self-consistent approximation

The following equations are anisotropic SCA, which are used to calculate the elastic tensor. These equations are the same as equations (27) in Hornby et al (1994).

\[
\mathbf{C}^{\text{a}} = \frac{1}{8\pi} \sum_{n=1}^{N} v_p (\mathbf{I} + \frac{\partial}{\partial n} (\mathbf{C}^{\text{a}} - \mathbf{C}^{\text{a}}))^{-1} \sum_{p=1}^{N} v_p (\mathbf{I} + \frac{\partial}{\partial n} (\mathbf{C}^{\text{a}} - \mathbf{C}^{\text{a}}))^{-1}^{-1} \mathbf{G}_{ijkl} = \frac{1}{8\pi} (\mathbf{G}_{ijkl} + \mathbf{G}_{ijkl}),
\]  

(A.1)

where $\mathbf{C}^{\text{a}}$ is in (A.1) is the estimated SCA result and the expression may be solved iteratively. Each $n$ and $p$ indicates an inclusion phase with volume fraction $v_n$. $\mathbf{G}$ in (A.1) controls the shape for each inclusion and can be defined by (A.2). Equations for $\mathbf{G}_{ijkl}$ can be found in Bandyopadhyay (2009).

Anisotropic differential effective medium

The following equations are anisotropic DEM, where $v, I$ and $G$ are as the same term as in equation (A.1). Unlike SCA, DEM is not a symmetry theory. $\mathbf{c}$ is the inclusion phase which needs to add into background material successively with an infinitesimal sub-volume.

\[
\frac{d}{dv} (\epsilon^{\text{DEM}}(v)) = \frac{1}{(1 - v)} (\epsilon^i - \epsilon^{\text{DEM}}(v)) K^{ij}(v) \epsilon^{\text{DEM}}(v) \quad (A.3)
\]

\[
K = [\epsilon (I + \mathbf{G} (\epsilon' - \epsilon))]^{-1} \quad (A.4)
\]

Bond transform and Voigt–Reuss–Hill average

The following equations are Voigt–Reuss–Hill (VRH) average for a disordered assembly of elastically anisotropic crystallites. All orientation can be covered by $\theta$ and $\phi$. $\theta$ is defined by the angle between crystallite symmetry axis and the composite symmetry axis, and $\Phi$ is the azimuth of the block. $\epsilon^V$ and $\epsilon^R$ are the stiffness and compliance for the composite. $\epsilon^a$ and $\epsilon^b$ are the stiffness and compliance for each block. $D(\theta)$ is the distribution function which control the probability for each rotated block. (A.8) is the Hill average (Hill 1952) which is based on the average of (A.5) and (A.7). These equations were the same as equations (36), (37), (38) and (39) in Hornby et al (1994).

\[
\epsilon^V = \frac{1}{2\pi} \int_0^{2\pi} \int_0^{\pi/2} D(\theta) \epsilon^a(\epsilon, \Phi) d\theta d\Phi \quad (A.5)
\]

\[
\int_0^{\pi/2} D(\theta) d\theta = 1 \quad (A.6)
\]

\[
\epsilon^R = \frac{1}{2\pi} \int_0^{2\pi} \int_0^{\pi/2} D(\theta) \epsilon^b(\epsilon, \Phi) d\theta d\Phi \quad (A.7)
\]

\[
\frac{\epsilon_{\text{VRH}}}{2} = \epsilon^V + (\epsilon^R)^{-1} \quad (A.8)
\]
\[ L_T = \begin{bmatrix} \cos \Phi & -\sin \Phi & 0 \\ \sin \Phi & \cos \Phi & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (A.12) \]

**Porosity effect of Xu’s model**

We handle the pore space of our model in the same way of Xu (2010). The total pore space is divided into three parts: clay-related pores, sand-related pores and micro-cracks (equation (A.13)).

\[ \phi_T = \phi_{\text{Clay}} + \phi_{\text{sand}}^{\text{iso}} + \phi_{\text{Crack}} \quad (A.13) \]

The volume of clay-related and sand-related pores can be estimated using normalized shale volume (A.14), and the porosity of cracks can be estimated based on an empirical relation between overburden stress and crack porosity (A.15).

\[ \phi_{\text{Clay}} = V_h \phi_T \quad (A.14) \]

\[ \phi_{\text{Crack}} = \phi_{\text{init}} e^{-\lambda \phi}. \quad (A.15) \]

All the pore types are added to the mineral background simultaneously based on the method proposed by Xu et al (2010). Xu’s method adds a small portion of all pore types proportionally at each iteration which avoid the asymmetry problem resulting from the order problem of DEM.

The clay-related pores and micro-cracks are assumed to be isolated and the sand-related pores are connected. The high frequency assumption of DEM can be used to model the isolated clay pores, and the capillary pressure in clay pores is lower than that of sand pores Xu et al (2010), wet pores are added into mineral using DEM to model the clay-related pores and micro-cracks. In terms of communicated sand-related pores, DEM is firstly used to build the dry frame and anisotropic Brown–Korring equation are introduced to model the saturated rock.

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