Appendix B

Rock physics modeling

I model the shale anisotropy from three aspects: mineral anisotropy of the rock constituents, compaction effect on the particle alignment, and the transition from smectite to illite due to compaction and temperature. To combine the anisotropic shale (clay) and the isotropic sand (quartz), I investigate two different effective-media models: the suspension model which and the lamination model. The suspension model simulates quartz as spherical inclusions in the clay background. The lamination model assumes thin layering effects between sand and shale.

Mineral anisotropy

We assume shales have three end-member mineral constituents: smectite, illite and quartz. The elastic properties are listed in Table B.1. The values of the smectite elasticity are the anisotropic elasticity values for a Cretaceous shale (Hornby et al., 1994). These approximated values are used as an end member when pure shale is fully compacted. Anisotropic elasticity for illite (muscovite) comes from work by Wenk et al. (2007). Similar to smectite, although the elasticity of a quartz crystal may be anisotropic, we assume isotropic quartz to approximate pure sand as an end-member in the rock.

Mineral	ρ (g/cc)	v_v (km/s)	v_s (km/s)	ϵ	δ	γ
Smectite	2.4	3.075	1.5	0.255	-0.05	0.48
Illite	2.4	4.94	2.6	1.02	0.	1.68
Quartz	2.65	6.0	4.0	0.	0.	0.

Table B.1: End-member mineral elastic properties.

Smectite to illite transition

The transition from smectite to illite is a common mineralogical reaction during burial diagenesis of shale. Many studies (e.g., Hower et al. (1976)) have shown that this transition reaction is controlled by the temperature in the subsurface. In this paper, we follow the work of Bachrach (2010a) to calibrate the percentage of illite P_I to the temperature T as follows:

$$P_I(T) = 0.5 + 0.5 \tanh(\frac{T - T_t}{2\sigma_t}), \tag{B.1}$$

with T_t as the transition temperature and σ_t as the length of the transition window. Reference values $T_t = 58°C$ and $\sigma_t = 60°C$ are from the work of Freed and Peacor (1989).

Preferred orientation distribution of clay mineral

Preferred orientation of the clay minerals is another important factor to the shale anisotropy (Hornby et al., 1994; Sayers, 2004). When initially deposited, mineral domains are oriented in random directions. In this case, even though an individual mineral domain can be anisotropic, the effective medium with randomly oriented domains is isotropic. During maximum compaction, all the mineral domains are fully aligned, which produces the effective medium with maximum anisotropy.

According to Bandyopadhyay (2009), the Voigt averaged stiffness coefficients C^a_{ij}

are

$$
\begin{aligned}
C_{11}^{a} &= L + 2M + \frac{4\sqrt{2}}{105}\pi^{2}(2\sqrt{5}a_{3}W_{200} + 3a_{1}W_{400}); \\
C_{33}^{a} &= L + 2M - \frac{16\sqrt{2}}{105}\pi^{2}(\sqrt{5}a_{3}W_{200} - 2a_{1}W_{400}); \\
C_{12}^{a} &= L - \frac{4\sqrt{2}}{315}\pi^{2}(2\sqrt{5}(7a_{2} - a_{3})W_{200} - 3a_{1}W_{400}); \\
C_{13}^{a} &= L + \frac{4\sqrt{2}}{315}\pi^{2}(\sqrt{5}(7a_{2} - a_{3})W_{200} - 12a_{1}W_{400}); \\
C_{44}^{a} &= M - \frac{2\sqrt{2}}{315}\pi^{2}(\sqrt{5}(7a_{2} + a_{3})W_{200} + 24a_{1}W_{400}); \\
C_{66}^{a} &= \frac{< C_{11} - C_{12} >}{2},
\end{aligned}
\tag{B.2}
$$

where

$$
\begin{aligned}
a_{1} &= C_{11} + C_{33} - 2C_{13} - 4C_{44}; \\
a_{2} &= C_{11} - 3C_{12} + 2C_{13} - 2C_{44}; \\
a_{3} &= 4C_{11} - 3C_{33} - C_{13} - 2C_{44}; \\
L &= \frac{1}{15}(C_{11} + C_{33} + 5C_{12} + 8C_{13} - 4C_{44}); \\
M &= \frac{1}{30}(7C_{11} + 2C_{33} - 5C_{12} - 4C_{13} + 12C_{44}),
\end{aligned}
\tag{B.3}
$$

with C_{ij} as the stiffness coefficients of the individual domain. The exponents W_{200} and W_{400} define the compaction rate. We use the porosity as an indicator for compaction (Bachrach, 2010a).

$$
\begin{aligned}
W_{200}(\phi) &= W_{200}^{\max}(1 - \phi/\phi_{0})^{m}, \\
W_{400}(\phi) &= W_{400}^{\max}(1 - \phi/\phi_{0})^{n},
\end{aligned}
\tag{B.4}
$$

with ϕ as the porosity at depth and ϕ_0 as the critical porosity. The choice of exponents m and n has not been well studied. We refer to Bachrach (2010a) and let both parameters vary between 0.5 and 2.

Suspension model: Anisotropic differential effective medium

One way to model sandy shales is to model quartz as an inclusion in the clay background. We use the anisotropic differential effective medium (DEM) method (Hornby et al., 1994) as implemented by Bandyopadhyay (2009). This process begins with an effective background shale with $\phi = 50\%$ modeled by self-consistent approximation (Berryman, 1980b,a), and it models the effective properties at other values of ϕ by successive operations of removing an infinitesimal subvolume of host material and replacing it with a corresponding subvolume of quartz. At each successive increment of components, the previous step is taken as the host material.

Lamination model: Backus average

At depth, seismic wavelengths can get as large as a few hundred meters. These long-wavelength seismic waves cannot resolve individual layers, but instead they interact with the subsurface as a single averaged medium. Elastic properties of an effective medium composed of fine-scale laminations of sand and shale can be described by the Backus average. We assume the sand layer contains pure sand and the shale layer contains pure smectite and illite. Backus (1962) showed that the elastic constants of the effective medium can be obtained by the elastic constants of the individual layers as follows:

$$\begin{aligned}
C_{11} &= < c_{13}/c_{33} >^2 / < 1/c_{33} > - < C_{13}^2 > + < c_{11} >; \\
C_{12} &= C_{11} - < c_{11} > + < c_{12} >; \\
C_{13} &= < c_{13}/c_{33} >^2; \\
C_{33} &= < 1/c_{33} >^{-1}; \\
C_{44} &= < 1/c_{44} >^{-1},
\end{aligned} \tag{B.5}$$

where $< . >$ indicates the averages of the enclosed properties weighted by their volumetric proportions. The volumetric proportions for each lithological components are calculated from the shale content and the percentage of illite. These enclosed properties can be averaged values over orientation distribution functions for shales.

Workflow

Our anisotropic rock physics modeling follows the workflow described here:

- Compute the percentage of illite in the rock, given a temperature model.
- Compute the average stiffness coefficients for smectite and illite, given a porosity model.
- Compute the volumetric percentage for each mineral phase, given a volumetric percentage of shale.
- Compute the stiffness coefficients using the suspension model or the lamination model.

At each instance of the modeling, the key parameters: ϕ_0, exponents m and n, T_t, and σ_t are varied within a certain range. Therefore, an assembly of models are obtained. These models will be the source of the prior rock physics covariance.