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Kerogen to oil conversion in source rocks. Pore-pressure build-up and effects on seismic velocities

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ABSTRACT

The aim of this work is to obtain a model for source rocks relating to kerogen–oil conversion and pore pressure to seismic velocity and anisotropy. The source rock is described by a porous transversely isotropic medium composed of illite/smectite and organic matter. The rock has a very low permeability and pore-pressure build-up occurs. We consider a basin-evolution model with constant sedimentation rate and geothermal gradient. Kerogen–oil conversion starts at a given depth in a volume whose permeability is sufficiently low so that the increase in pressure due to oil generation greatly exceeds the dissipation of pressure by flow. Assuming a first-order kinetic reaction, with a reaction rate satisfying the Arrhenius equation, the kerogen–oil conversion fraction is calculated. Pore-pressure changes affect the dry-rock stiffnesses, which have an influence on seismic velocities. The properties of the kerogen–oil mixture are obtained with the Kuster and Toksöz model, assuming that oil is the inclusion in a kerogen matrix. We use Gassmann's equations generalized to the anisotropic case to obtain the seismic velocities of the source rock as a function of depth, pressure and oil saturation. The procedure is to obtain the dry-rock stiffnesses by assuming a Poisson medium for the mineral material constrained by the physical stability conditions at the calibration confining pressures.

The example considers a sample of the North-Sea Kimmeridge shale. At a given depth, the conversion increases with increasing geothermal gradient and decreasing sedimentation rate, and the porosity increases with depth due to the conversion. As expected, the horizontal velocities are greater than the vertical velocities and the degree of anisotropy increases with depth. The analysis reveals that the vertical P-wave velocity is the main indicator of overpressure.

1. Introduction

Oil can be generated from kerogen-rich source rocks and flow through a carrier bed to a sandstone reservoir rock. Excess pore-fluid pressures are generated when the rate of volume created by the transformation of oil to gas is more rapid than the rate of volume loss by fluid flow. Research conducted by Vernik on petroleum source rocks (Vernik and Nur, 1992; Vernik, 1994, 1995; Vernik and Landis, 1996) indicates that strong velocity anisotropy is associated with the presence of organic matter.

Berg and Gangi (1999) derived a procedure to obtain the conversion of kerogen to oil and the related pressure buildup in a source rock, based on the following assumptions. i) The permeability of the rock is small so that the pore-pressure buildup by the conversion is much faster than its dissipation by pore-fluid flow. ii) The stress state is isotropic and the rock breaks when the pore pressure equals the confining pressure. iii) One reaction rate is required for the conversion. Carcione (2000) used this model to calculate the excess pore pressure as a function of the fraction of kerogen converted to oil. The conversion ratio is computed as a function of time, for a given sedimentation rate and geothermal gradient, using the Arrhenius equation. The excess pore pressure due to the conversion with burial time is derived by balancing mass and volume changes in the pore space (see also Carcione and Gangi, 2000a,b).

Hydrocarbon source rocks are transversely isotropic media composed of organic matter (kerogen and oil) and illite layers. Vernik in his works and Carcione (2000) used Backus averaging to model the seismic velocities. Here, we use a different approach based on Gassmann equations for an anisotropic frame and an isotropic solid pore infill (kerogen–oil) (Ciz and Shapiro, 2007). The effective properties of illite are obtained by assuming an isotropic Poisson medium constrained by the physical stability conditions applied to the elastic constants of the dry frame, which are obtained by inversion of Gassmann's equations. The method is applied to the Kimmeridge shale, from data provided by Vernik (1995). This is the novel part of this work and to our knowledge it is the first application of Gassmann theory and its "fluid-substitution" version (i.e., inverse Gassmann's equation) to describe the properties of organic shales. This is possible to the generalization of the pore-infill to a solid material. Note that the

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models based on Backus averaging were developed before the introduction of Ciz and Shapiro (2007) generalization of Gassmann's equations. This new theory, in its isotropic version, has already been used to describe the properties of rocks filled with heavy oil, which has a non-negligible shear modulus (Das and Batzle, 2008).

In the following, K and μ, and ρ indicate bulk and shear moduli, and density, and the indices m, s, o, k and if denote dry matrix (skeleton), solid grain (clay), oil, kerogen and pore infill (kerogen–oil mixture), respectively. Moreover, $c_{IJ}=c_{ijkl}$ is the two-index notation for stiffnesses (Helbig, 1994), s_{IJ} and s_{ijkl} for compliances, and ϕ denotes porosity or proportion of a given material.

2. Kerogen to oil conversion

Firstly, we introduce some useful definitions about the different pressures considered in this work. *Pore pressure*, also known as formation pressure, is the in situ pressure of the fluids in the pores. The pore pressure is equal to the *hydrostatic pressure* when the pore fluids only support the weight of the overlying pore fluids (mainly brine). The *lithostatic* or *confining pressure* is due to the weight of overlying sediments, including the pore fluids. Fractures perpendicular to the minimum compressive stress direction appear for a given pore pressure, typically 70–90% of the confining pressure. In this case, the fluid escapes from the pores and pore pressure decreases. A rock is said to be overpressured when its pore pressure is significantly greater than hydrostatic pressure. The difference between pore pressure and hydrostatic pressure is called *differential pressure*. Acoustic and transport properties of rocks generally depend on *effective pressure*, a combination of pore and confining pressures (e.g., Carcione, 2007). Various physical processes cause anomalous pressures on an underground fluid. The most common causes of overpressure are compaction disequilibrium and cracking, i.e., oil to gas conversion (Carcione and Gangi, 2000a,b).

Let us assume a source rock at depth z. The lithostatic pressure for an average sediment density of $\overline{\rho}$ is equal to $p_c=\overline{\rho}gz$, where g is the acceleration of gravity. On the other hand, the hydrostatic pore pressure is approximately $p_{\mathrm{H}}=\rho_w gz$, where ρ_w is the density of water.

For a constant sediment burial rate, S, and a constant geothermal gradient, G, the temperature variation of a particular sediment volume is

$$T=T_0+Gz,\ z=St, \tag{1}$$

with a surface temperature T_0 at time $t=0$. Typical values of G range from 20 to 30 °C/km, while S may range between 0.02 and 0.5 km/m.y. (m.y. = milion years).

Assume that at time t_i, corresponding to depth z_i, the shale contains kerogen and that the volume is “closed”. That is, the permeability is sufficiently low so that the rate of pressure increase due to oil generation greatly exceeds the dissipation of pressure by flow. Pore pressure excess is intended to be above hydrostatic.

2.1. Kerogen–oil generation rate

The mass of convertible kerogen changes with time t at a rate proportional to the mass present. Assuming a first-order kinetic reaction (Luo and Vasseur, 1996; Pepper and Corvi, 1995)

$$\frac{dM_k}{dt}=-r_k(t)M_k(t) \tag{2}$$

or

$$M_k(t)=M_{ki}\ exp\left[-\int_{t_i}^{t}r_k(t)dt\right], \tag{3}$$

where $r_k(t)$ is the reaction rate, $M_k(t)$ is the mass of convertible kerogen at time t and M_{ki} is the initial kerogen mass. The fraction of kerogen converted to oil is $F(t)=[M_{ki}-M_k(t)]/M_{ki}$:

$$F(t)=1-\ exp\left[-\int_{t_i}^{t}r_k(t')dt'\right]\equiv 1-\ exp[-\Phi(t)]. \tag{4}$$

The reaction rate follows the Arrhenius equation (e.g., Luo and Vasseur, 1996)

$$r_k(t)=A\ exp[-E/RT(t)], \tag{5}$$

where E is the kerogen–oil activation energy, $R=1.986$ cal/mol °K is the gas constant, A is the kerogen–oil reaction rate at infinite temperature, and $T(t)$ is the absolute temperature in °K given by

$$T=T_0+Ht,\ H=GS. \tag{6}$$

With this temperature dependence, the integral $\Phi(t)$ becomes

$$\Phi(t)=\int_{t_i}^{t}r_k(t')dt'=\frac{A}{H}\int_{T_i}^{T}exp(-E/RT')dT',\ T_i=T_o+Ht_i \tag{7}$$

or

$$\Phi(t)=\frac{A}{H}\left[T\int_1^\infty exp(-Ex/RT)\frac{dx}{x^2}-T_i\int_1^\infty exp(-Ex/RT_i)\frac{dx}{x^2}\right]. \tag{8}$$

For values of E/RT greater than 10, the exponential integral can be approximated by Gautschi and Cahill (1964, pp. 248, Table 5.5)

$$\int_1^\infty exp(Ex/RT)\frac{dx}{x^2}\cong\frac{exp(-E/RT)}{2+E/RT}, \tag{9}$$

with an error of 1.3% or less. Then, the integral Φ becomes

$$\Phi(T(t))=\frac{A}{H}\left[\frac{T\ exp(-E/RT)}{2+E/RT}-\frac{T_i\ exp(-E/RT_i)}{2+E/RT_i}\right]. \tag{10}$$

2.2. Kerogen to oil conversion versus excess pressure

Excess pore pressure (overpressure) is the main mechanism for oil migration. This phenomenon occurs mainly in low permeability rocks (e.g., compacted shales), where high-density organic matter, such as kerogen, is transformed to less dense fluids (oil and gas), with a rate exceeding the rate of volume loss by flow. In order to obtain a simple formula for computing the excess pore pressure as a function of the volume fraction of kerogen transformed to oil, the following assumptions are made: i) no loss of fluid from the source-rock pore volume (negligible permeability); ii) the compressibilities are independent of pressure and temperature — in particular the pore-space one is that at the initial pore pressure; iii) the initial pore volume contains only convertible kerogen, since water content is very small and is part of the matrix (which contains hydrated smectite in part); iv) negligible conversion of oil to gas; v) the confining pressure is approximately constant during oil generation, i.e., the reaction rate is high enough such that the overburden pressure does not change significantly during the conversion process; and vi) volume changes with temperature are negligible.

As stated by Vernik (1994), horizontal micro-cracks may be initiated and kept open during the conversion process. Our model assumes that permeability is so low that the reaction is local at a microscopic scale. In this sense, the “closed system” assumption can be a rough approximation in some cases, since it may imply an anomalous increase in porosity (approximately 10% in the examples given here). Therefore, a more realistic model should consider