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A molecular informed poroelastic model for organic-rich, naturally occurring porous geocomposites



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ABSTRACT

Molecular simulation results on organic maturity (mature and immature kerogen as the two asymptotic cases) are introduced into a continuum micromechanics based model for organic-rich shales. Through a fundamental functional relationship that constrains microporous kerogen density and elasticity variable spaces and within the framework of effective media theory; the model bridges the gap between asymptotic cases of organic maturity with texture as the overriding theme, specifically a matrix/inclusion (Mori–Tanaka) texture for immature systems and a granular (self-consistent) texture for mature ones. The utility of the molecular results merged into a continuum framework is demonstrated by estimating kerogen's microporosity (<2 nm) from nanoindentation measurements. The effect of burial and diagenetic processes on the effective poroelasticity of these porous, naturally occurring geocomposites are captured by introduction of imperfect interfaces. Finally, the performance of the model is fully characterized by ranking the normalized contribution of uncertainty of input to the overall behavior and parameters of interest to geophysicists and geomechanicians such as degree of anisotropy and *in situ* stresses.

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1. Introduction

Due to their abundance, organic-rich shales are playing a critical role in re-defining the world's energy landscape and in re-formulating the global geopolitics. However, technological challenges and environmental concerns continue to contribute to the slow growth of organic-rich shale exploration and exploitation worldwide. The highly heterogeneous nature and anisotropic behavior (mechanical and transport) of these porous organic/inorganic composites leave many open questions regarding their characterization, modeling and engineering design. Our objective is to link organic maturity and its elasticity to the effective elastic and poroelastic behavior of these intricate, naturally occurring geocomposites with texture as the overriding theme. The significant body of literature on modeling shales and organic-rich shales (see e.g. Vernik and Nur, 1992; Hornby et al., 1994; Ulm et al., 2004; Ortega et al., 2009b; Vernik and Kachanov, 2010; Sayers, 2013; Khadeeva and Vernik, 2014); does not explore the effect of organic maturity on the overall poroelastic behavior of these source rocks. In addition, the elasticity and the density of the organics are often assumed *a priori*; failing to account for variations in structural, physical and chemical properties of these organics.

In a hypothesis testing approach, we attribute the first-order contribution of organic maturity on overall elasticity for low total organic carbon (TOC ≤ 1 mass%) shales to a texture effect while for high TOC systems, kerogen elastic properties assume

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a role of first-order nature. Assuming all organics to be microporous kerogen, we utilize a functional relationship obtained from molecular simulations on these microporous organics (Bousige et al., 2015) to constrain kerogen stiffness and its density variable spaces; avoiding any assumptions *a priori* for these parameters. The simulations of Bousige et al. (2015) were performed on re-constructed microporous kerogen samples and thus the kerogen phase referred throughout this work is a microporous organic solid. The elastic and the fracture behavior of three re-constructed microporous kerogen samples with different levels of maturity using a hybrid experimental-simulation technique were explored by Bousige et al. (2015). Their results suggest that kerogen's Poisson's ratio has a low sensitivity with respect to its density and the state of maturity. A nearly constant ($\nu^{\text{kerogen}} \approx 0.25$) Poisson's ratio from molecular simulations of Bousige et al. (2015) leaves one degree of freedom associated with the isotropic elasticity of kerogen that is constrained through a fundamental functional relationship with the density of kerogen, ρ^{kerogen} (see Fig. 6). The low sensitivity of ν^{kerogen} to the state of maturity seems to be a consequence of the amorphous structure of kerogen and the randomness of the network that connects these organic macromolecules.

As an application we estimate kerogen's microporosity from elastic measurements, in this case instrumented nanoindentation data. The incorporation of the molecular simulation results into a mean field based framework shows promise in providing an unprecedented insight into subsurface rock properties from elastic based measurements e.g. seismic and sonic wave velocities.

Lastly, we employ Spearman's partial rank correlation coefficient (SPRCC) to fully characterize the sensitivity of our model to uncertainty in input parameters. The results can be of interest to geoscientists to better manage confidence in their calculations by characterizing parameters with the highest contribution.

2. Theoretical tools

2.1. Homogenization and inclusion based effective estimates

The fourth-order homogenized stiffness tensor, \mathbb{C}^{hom} , associated with a defined representative elementary volume, *rev*, denoted by Ω , can be obtained from (Zaoui, 2002):

$$\mathbb{C}^{\text{hom}} = \langle \mathbb{C}^r(\underline{x}): \mathbb{A}^r(\underline{x}) \rangle_{\Omega} \quad \forall \underline{x} \in \Omega \quad (1)$$

where $\langle \dots \rangle_{\Omega}$ implies volume averaging over Ω and $\Omega = \Omega^1 \cup \Omega^2 \cup \Omega^3 \cup \dots \cup \Omega^r$ where Ω^r represents the *r*th subdomain, all mutually exclusive. The scale separability condition requires the characteristic size of a micro-homogeneous phase in Ω , denoted by *d*, to be much smaller than the characteristic length of the *rev*, ℓ , for homogenization (Zaoui, 2002). \mathbb{C}^r is the stiffness tensor of the *r*th micro-homogeneous phase and \mathbb{A}^r is the fourth-order strain localization tensor. Due to Eshelby's celebrated solution (Eshelby, 1957), in linear elasticity one can define the strain concentration tensor for phase *r*, \mathbb{A}^r , as follows (Dormieux et al., 2006):

$$\mathbb{A}^r = [\mathbb{I} + \mathbb{P}: (\mathbb{C}^r - \mathbb{C}^0)]^{-1}: \left\langle [\mathbb{I} + \mathbb{P}: (\mathbb{C}^r - \mathbb{C}^0)]^{-1} \right\rangle_{\Omega}^{-1} \quad (2)$$

where $\mathbb{I} = I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the fourth-order identity tensor, \mathbb{C}^0 denotes the background matrix stiffness tensor, and \mathbb{P} is the fourth-order Hill concentration tensor. The generalized expression for Hill concentration tensor reads (Zaoui, 2002):

$$P_{ijkl} = - \left(\frac{\partial^2}{\partial x_j \partial x_l} \int_{\Omega} G_{ik}(\underline{x} - \underline{x}') d\Omega \right)_{(ij)(kl)} \quad (3)$$

with $(ij)(kl)$ implying indices symmetrization and $G_{ij}(\underline{x} - \underline{x}')$ representing the second order Green's tensor for a generalized linear, elastic, anisotropic medium that characterizes displacement at point \underline{x} due to a Dirac delta type point force at \underline{x}' . Hill concentration tensor is related to Eshelby tensor, \mathbb{S}^{Esh} , in the following way:

$$\mathbb{S}^{\text{Esh}} = \mathbb{P}: (\mathbb{C}^0)^{-1} \quad (4)$$

There are different ways to approximate Eq. (2) since aside from volume fractions, statistical distribution of higher order textural parameters is almost never available for a random media. The two approximation schemes, with some physically meaningful interpretations, are the self-consistent and the Mori–Tanaka. The self-consistent approximation scheme was introduced and developed by Hershey (1954), Kroner (1958), Budiansky (1965) and Hill (1965). In the self-consistent scheme, \mathbb{C}^0 in Eq. (2) is set equal to \mathbb{C}^{hom} resulting in an implicit expression. This implies that no particular phase plays a dominant role in contributing to the effective stiffness of the composite. The Mori–Tanaka approximation scheme was initially proposed by Mori and Tanaka (1973) and further developed by Benevise (1987). The Mori–Tanaka approximation scheme can be achieved by setting \mathbb{C}^0 in Eq. (2) equal to \mathbb{C}^M , where \mathbb{C}^M is the stiffness of the dominant matrix phase. Mori–Tanaka is often associated with a “swiss-cheese”/matrix-inclusion texture.

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