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BRIEF NOTE

A model of fracture-facilitated flow of hydrocarbons from petroleum source rock

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Abstract We study the processes by which petroleum originates in source rock and generates a transport path enabling some of it to leave. We show that diffusion through the source rock is too slow to account for the migration of petroleum. However when kerogen converts into petroleum within pores, it expands, and this expansion is sufficient to fracture the rock around the pores. Thus the transport of petroleum depends on whether these fractures connect up to form a macroscopic transport path. We develop a simulation tool that lets us study pressurized fluid in disk-shaped domains which expand and fracture the surrounding material. Examining pairs of pressurized pores, we obtain a lower limit for critical porosity in shale rock, $\phi_{\text{crit.}} = 0.15$. When kerogen saturation exceeds this value, long-range transport paths become possible. This critical porosity is comparable to the porosities observed in immature shales.

Keywords Petroleum transport · Computational physics · Fracture · Fluid dynamics

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1 Introduction to shale and petroleum reservoirs

The source rocks from which petroleum originate are frequently so impenetrable that fluid flow across centimeters is impossible, even over tens of millions of years, and for realistic pressure gradients. Thus, what seems to be required is a mechanism for hydrocarbon expulsion that naturally varies between allowing free flow and no flow at all.

While we do not believe that we propose the only possible mechanism, we find that microfractures driven by overpressure as petroleum forms have the potential to produce transport networks that will allow petroleum to move over long distances. However, whether the cracks link up or not depends critically on geometric details, such as the size and density of petroleum-rich regions. This allows us to explain how regions with complete expulsion and complete trapping can exist in close proximity.

It is generally accepted that the driving force for petroleum expulsion comes from the conversion of kerogen into the lower-density liquids, bitumen, then petroleum and finally gases (mostly methane), which increases pore pressure unless they are released. We will refer to this process as petroconversion. Kerogen, bitumen and petroleum are all liquid inside shale, and are almost incompressible, petroleum having a compressibility of $\sim 3\times10^{-9}$ Pa (Okotie and Ikporo 2019).

Fracture networks have often been suspected to play a role in petroleum expulsion (Gale et al. 2014; Haider

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et al. 2022). Fracture mechanisms are known to play an important role in geological fluid transport. In this paper, we will investigate a mechanism wherein pre-oil solid bitumen creates a transport pathway by expanding until it cracks the surrounding rock. If cracked pores are sufficiently close, the fractures join together and create a connected pathway for long-distance transport.

2 Expansion, pressure, and fracture pathways

Leythauser et al. (1982) states: "Due to an exponential decrease of the diffusion coefficient with increasing carbon number, the diffusive flux rate of petroleum-range hydrocarbons is so low that this mechanism probably does not contribute significantly to primary migration of petroleum-range hydrocarbons." England et al. (1987) agree with this conclusion and further posit that a bulk flow mechanism must be responsible for petroleum migration. Inan et al. (1998) write that the actual mechanism of petroleum migration out of source rock is "…a fundamental question still awaiting the right answer."

If one considers the length of petroleum molecules, which is on the order of nanometers (Chen et al. 2011), in relation to characteristic length scale for diffusion channels in shale, one sees why diffusion rates for molecules can drop exponentially as their length increases. The permeability of shale is approximately 10 nanodarcy, which in SI units is 9.9×10^{-21} m^2. This corresponds to a characteristic length of an Angstrom. Noting that the wall-facing cross-section of petroleum molecules exceeds this length scale, we do not expect petroleum trapped in shale to be governed by conventional measures of permeability, which are obtained from diffusion of gases.

Since the effective shale permeability to petroleum is zero, we explore here a specific mechanism, which is that bulk flow is achieved via the creation of inter-pore fracture networks resulting from the pressure that is generated during the process of petroconversion. Haider and Patzek (2020) anticipated the idea of micron-scale fracture networks aiding the migration of hydrocarbons.

In order to determine whether fracture is a possible mechanism by which petroleum migrates, we need to determine the pore pressure in shale due to petroconversion and determine if this pressure is great enough to overcome the surface energy of shale. During the process of petroconversion, kerogen converts to petroleum. The conversion from kerogen to petroleum is a complex process that occurs in fits and pauses, with a highly non-linear time dependence. However, in order to facilitate this study we will assume that the conversion takes place linearly in time. Kerogen has a density of 1.35 grams per cubic centimeter, and petroleum a density of 0.8 (Stankiewicz et al. 2015). This represents a 41% decrease in density, which in the case of the Jafurah basin occurred over the course of roughly 10 million years (Speight 1999; Haider et al. 2022). In order to calculate the end-time overpressure in shale due to petroconversion, we use:

$$P(t) = \frac{1}{C_0} \ln\left(\frac{\Delta\rho}{\rho_0}\frac{t}{t_{\max}} + 1\right) \tag{1}$$

where $\Delta\rho$ is the change in density during petroconversion, ρ_0 is the initial density (the density of kerogen), $t_{\max}$ is the time at which petroconversion ceases, and C_0 is the compressibility of petroleum. Substituting previously given values, we arrive at an end-time overpressure of approximately 100 MPa, cf. Haider et al. (2022).

Consider a spherical pore filled with pressurized fluid: the stress parallel to the surface of the pore will be $P/2$. Using the Irwin relation between fracture toughness and energy due to strain, one readily arrives at the expression

$$a \approx \frac{\Gamma Y}{\pi P^2}. \tag{2}$$

Here a is the smallest surface crack that can be driven, P is pressure, Y is Young's modulus and Γ is fracture toughness. Taking fracture toughness to be approximately 100 J/m^2, and Young's modulus to be 1 GPa, we find that 100 MPa can drive an approximately 1 micron long surface crack (Marder et al. 2015). This indicates that pores of less than the micron scale are unlikely to fracture due to the pressure generated from petroconversion. However, pores at or above this scale will fracture under such conditions.

3 Basis of simulation

Organopores can fracture under pressure resulting from petroconversion. However, this is not sufficient to demonstrate that petroleum can migrate away from source rock via fracture networks. In order to demonstrate this, we must show that fractures emanating from

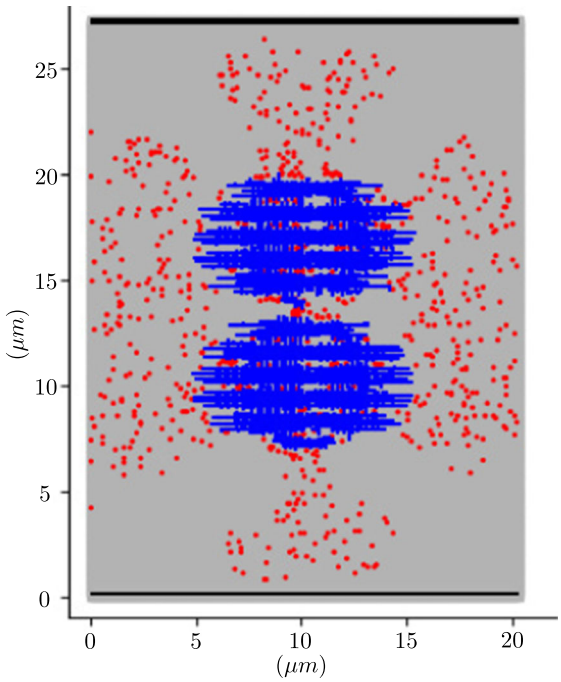

Fig. 1 Two meta pores after 10 Myr, still barely disconnected. Blue regions indicate kerogen filled organopores, whereas the grey represents regions of shale. Meta pores do not connect nearly as readily when facing length-wise. Red dots represent places where the lattice has fractured but not filled with fluid

adjacent pores can connect, allowing for fluid flow between them. We use a numerical model to investigate how this connectivity emerges.

We model the real system (a pore filled with fluid that expands due to chemical change over time) as a pore filled with incompressible fluid injected everywhere over some length of time (10 million years). To do this, we began with a numerical model developed by Marder et al. (2015). This model was originally developed to study hydraulic fracturing of shale. In order to study the problem of organopore fracture due to internal pressure, we revised the model in order to accommodate different geometry, dynamics and scale.

The simulation describes two coupled physical phenomena—a solid that can deform elastically and fracture, and a pressurized fluid that flows inside open channels and fractures. The first of these phenomena is modeled as a square lattice of point masses connected by springs. These mass points compose the continuous space of the source rock's microscopic geometry, meaning that structures such as pores and fractures are composed of many individual mass points. Springs have spring constants which are tuned to the material properties of shale, subject to the addition of a small amount of random noise which mirrors the random anisotropy present in real rock. Noise also serves to add a stochastic element to our simulation, which produces varying results for the same input parameters. This variability allows us to perform statistics for a given geometry, rather than only exploring the deterministic solution to the special case in which the rock is completely isotropic.

The mass points obey Hookean dynamics, meaning force is proportional to displacement from nearest neighbors. The bonds between mass points, if overextended, snap and disappear, creating a PKN style fracture. A separate lattice of fluid channels bisects each adjacent mass, though points on this lattice only become filled with fluid if the bond connecting adjacent mass points is broken and adjacent points on the fluid channel contain fluid. Fluid inertia is neglected in accordance with the lubrication approximation. However, pressure is computed and exerts force on the mass points, leading to extension, eventually broken bonds and fracture. In this way, fractures occur, allowing mass points to move far apart, creating space for fluid transport. This in turn exerts elastic forces on the rest of the system, leading to continued deformation.

Specifically, the solid lattice obeys the following force law:

$$F_R = \sum_{R'} k_{\parallel}(\delta u_{R,R'} \cdot \mathbf{\Delta}_{R,R'}) \cdot \mathbf{\Delta}_{R,R'} + k_{\parallel}\delta u_{R,R'} + LP_{R,R'}\Delta_{R,R'} - \beta \dot{u}_{R,R'} \tag{3}$$

F_R is the force on a point R. R' represents all mass points adjacent (bonded with) R. $\mathbf{\Delta}_{R,R'}$ represents the vector difference between R and R' prior to any deformation. $\mathbf{u}_{R,R'}$ represents the vector difference between R and R' for the actual, potentially deformed, lattice. $P_{R,R'}$ is the pressure of any fluid channel between R and R'. L is the lattice spacing. β is a damping constant. Because vibrational modes of the lattice are of no importance, we set damping to a high arbitrary value. The extension δ between adjacent mass points at which bonds break is given by the equation $\delta = \sqrt{2\Gamma L/Y}$.

Young's modulus of shale rock is on the order of GPa, so we measure elastic moduli in GPa. The time required for petroconversion to finish is about ten million years, so we take 1 Mya to be the unit of time. Finally organopores are on the micron scale; therefore we take 1 μm to be the unit of length. These three

choices define the units of length, time, and energy in our dimensionless system.

In real shale rock, micron-scale organopores, which we will call "meta-pores" or "meta-bubbles", are comprised of roughly elliptical, slightly smaller micron-scale pores (which we will call "sub-pores" or "sub-bubbles"). We will use as our reference figure 5 from Cardott et al. (2015). We indicate the sub-bubbles minor and major axes as x and y, respectively. The meta-bubble radius will be indicated as before, as will the meta-bubble center-to-center spacing.

If we assume the sub-bubbles are arranged on a rectangular lattice with a surface-to-surface spacing of S, we can write down a formula for porosity which goes like:

$$\phi = \frac{\pi^2 r^2 xy}{a^2(2x + S)(2y + S)} \tag{4}$$

We use Eq. 4 when calculating the porosities stated in our results.

Our simulation explores two characteristic geometries. One involves two adjacent pores, oriented in such a way that their semi-minor axes are coincident. This arrangement is "length-to-length". The other geometry involves two adjacent pores with coincident semi-major axes. This arrangement is "end-to-end".

4 Simulation results

In order to capture the length scales present in shale, we performed simulations for 3 distinct meta-bubble sizes: 1.5, 3 and 6 microns in radius. For each simulation, initial porosity was calculated using Eq. 4.

The final configuration at 10.05 megayears (the step directly succeeding petroconversion end-time, as shown in Fig. 1) was then visually inspected to confirm whether the meta bubbles had in fact merged or not. The data were then divided into bins with a width three times the quotient of the total range of porosities studied and the square root of the total number of simulations studied. The mean and standard error of these bins were computed and plotted along with a piecewise cubic Hermite interpolating polynomial. The outcome is represented in Figs. 2 and 3. For end-to-end configurations, critical porosity is approximately 0.09. In the length-to-length configuration, critical porosity is approximately 0.24. Given that real shale consists of a mix of angles between pores, an appropriate value of critical porosity in the real case would be a geometric mean of the critical porosities determined in the cases studied—length-to-length geometry and end-to-

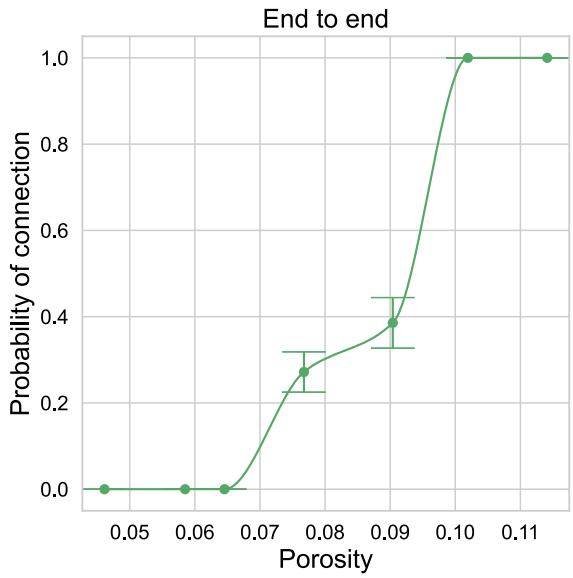

Fig. 2 Here are results from end-to-end configurations. The results from a total of 302 simulations are visualized here. 83 of these simulations used a meta-bubble radius of 6 microns; 127 used a meta-bubble radius of 3 microns; and 92 used a meta-bubble radius of 1.5 microns

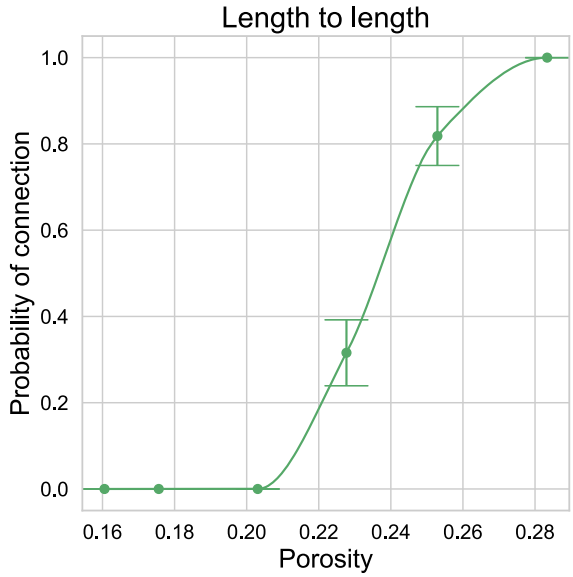

Fig. 3 Here are results from end-to-end configurations. The results from a total of 197 simulations are visualized here. 48 of these simulations used a meta-bubble radius of 6 microns; 101 used a meta-bubble radius of 3 microns; and 48 used a meta-bubble radius of 1.5 microns

end geometry. Therefore, our predicted lower limit for the critical porosity of shale is approximately 0.15.

The results of this work are qualitatively similar to those obtained by Haider et al. (2022), using a different approach.

5 Discussion

We conclude that fractures driven by pore overpressure can explain the migration of petroleum through seemingly impermeable rock. The mechanism is capable of creating transport paths of arbitrary length, and becomes active at porosities that are in range of those seen experimentally. The mechanism has another required property, which is that depending upon fine details at the micron scale, oil may either migrate or be trapped. The intent of our simulations is not to pin down the precise conditions under which this happens, but to show how this qualitative feature emerges as a consequence of reasonable assumptions in a simple model.

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