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1 **Microfracturing during primary migration in shales**

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13 14 **Abstract**

15 In several geological environments, chemical reactions are coupled to rock deformation and the
16 associated stresses induced locally interact with the far field loading. This is the case in
17 immature shales that undergo burial and diagenesis, where the organic matter evolves with
18 temperature into hydrocarbons which induces local volume expansion. At large scale, this
19 mechanism is responsible for the transport of hydrocarbons from source to reservoir rocks, a
20 process referred to as primary migration. However, how the interactions between local fluid
21 production, microfracturing, and transport are coupled remain to be understood. Here, we
22 analyze this coupling phenomenon by developing a discrete element model where the
23 generation of local overpressures occurring in kerogen patches is simulated, while the
24 surrounding rock is subjected to external loading. It is shown that, due to local fluid
25 overpressure; microfracturing occurs and brings the fluids to migrate through the medium. The
26 numerical results are confirmed by laboratory experiments where the network of microfractures
27 induced in an immature Green River shale sample heated under small differential stress was
28 imaged in three dimensions using X-ray microtomography. Moreover, the numerical
29 simulations identify that the state of differential stress and the initial kerogen distribution
30 constitute two key parameters that control the formation of the three-dimensional percolating
31 microfracture network and could thus explain primary migration in shale rocks.

32

33 **Keywords:** shale, microfracture, kerogen, X-ray tomography, Discrete Element Model

34

35 **Highlights**

36 - Kerogen maturation produces microfractures in shale rocks

37 - Microfractures form a percolating network

38 - Differential stress and spatial distribution of kerogen control the geometry of the final
39 microfractures network

40

41 **1. Introduction**

42 The coupled response of chemical reactions and deformation in rocks can induce the
43 development of localized damage in the form of connected microfractures or microporosity
44 which facilitate the circulation of fluids. These phenomena are observed in various geological
45 processes such as weathering and erosion of surface rocks ([Røyne et al., 2008](#); [Jamtveit and
46 Hammer, 2012](#)), hydration of the Earth's lower crust ([Peacock, 1993](#); [Jamtveit et al., 2000](#)),
47 dehydration of sediments in subduction zones ([Ulmer and Trommsdorff, 1995](#); [Saffer and
48 Bekins, 1998](#); [Brantut et al., 2012](#)), alteration of monuments by salt precipitation ([Noiriel et al.,
49 2010](#)), or the maturation of organic matter in source rock sediments ([Snarsky, 1961](#); [Tissot and
50 Welte, 1978](#); [England et al., 1987](#); [Hunt, 1990](#); [Lafargue et al., 1993, 1998](#); [Vernik, 1994](#);
51 [Rudkiewicz et al., 1994](#); [Kobchenko et al., 2011](#)). For the latter, the coupling between
52 maturation of the organic matter and creation of porosity by fracturing of the source rocks
53 during burial may lead to hydrocarbon escape towards a more porous reservoir, a process called
54 primary migration.

55 Shale rocks overlie or underlie most hydrocarbon-bearing reservoirs, forming cap rocks and
56 source rocks. They prevent fluids from escaping due to their low permeability and by a capillary
57 sealing mechanism controlled by the small pores ([Horsrud et al., 1998](#)). While the presence of
58 fractures in shales in outcrops and from cores through unconventional reservoirs has been

59 described (Gale et al., 2014), the presence of microfractures and microporosity at smaller scales,
60 that may control the overall permeability, is debated because of scarce observations (Gale et
61 al., 2014; Kalani et al., 2015, Ougier-Simonin et al., 2016). Sometimes, bitumen-filled
62 microfractures with chemical characteristics similar to decomposed kerogen are observed (Lash
63 and Engelder, 2005), in other cases the presence of sealed veins indicate that microfractures
64 were open at depth (Kalani et al., 2015). Moreover, microfractures control the long-term sealing
65 capacities of cap rocks, the expulsion of hydrocarbon during primary migration, and the
66 potential increase in permeability when reactivated by hydraulic fracturing. More generally, the
67 petrophysical properties of argillite rocks have fundamental implications, for example on their
68 frictional behavior in faults (Brantut et al., 2008) and in controlling their permeability (Holland
69 et al., 2006).

70 Kerogen maturation into oil and gas leads to a volume increase in the order of 10-20% at
71 standard pressure and temperature conditions. In many cases maturation takes place within the
72 internal porosity of kerogen flakes, which may indicate that expansion of the solid might be
73 another cause of microfracturing. Such overpressure mechanisms have been proposed to be
74 high enough to fracture the source rock (Pelet and Tissot, 1971; Vernik, 1994). When the
75 overpressure reaches a critical stress, microfractures starts to nucleate and propagate (Hunt,
76 1990; Capuano, 1993; Vernik, 1994; Jin et al., 2010). Propagating microfractures may then
77 coalesce and even get connected to pre-existing vertical fractures which would further facilitate
78 hydrocarbon primary migration (Fan et al., 2012).

79 Here, we study the process of primary migration coupled to microfracture development by a
80 combined experimental and numerical approach. The experimental component involves
81 imaging in three dimensions (X-ray tomography) of Green River shale samples that were heated
82 under small differential stress, in order to characterize the network of microfractures produced
83 during the maturation of organic matter (Kobchenko et al., 2011; Panahi et al., 2013). The
84 natural Green River shale rock contains kerogen organic matter which is present in the form of
85 sub-millimeter elongated ellipsoids distributed in the rock matrix. These patches, when
86 undergoing thermal maturation, act as local sources of overpressure due to the breakage of
87 shorter molecules from the very long chained molecules constituting the polymerized kerogen.
88 Such pressure variations can induce local microfracturing at the scale of the kerogen patches.
89 These fractures then grow and ultimately connect to each other in three-dimensions, spanning
90 the whole volume of the rock mass. In order to gain more insight into the process, we simulate

91 numerically the formation and propagation of these microfractures at the scale of kerogen
92 patches using a three dimensional model based on the discrete element method (Cundall and
93 Strack, 1979, Donzé and Magnier, 1993). The conditions under which these microfractures
94 become the preferred paths for fluid products and control primary migration are then discussed.

95 **2. Materials and methods**

96 **2.1 Experiments of shale maturation**

97 Two core samples of a Green River shale, that contains 5 wt. % type I kerogen, were heated to
98 390°C in pressure vessels for 48 hours to transform the kerogen into oil and gas. The rock is
99 made of quartz, clays, pyrite, and carbonate minerals and has a low porosity, close to 5% as
100 measured by helium gas adsorption method. This rock is an immature shale and previous
101 experiments have shown that kerogen maturation at atmospheric pressure can be performed at
102 temperatures in the range 300-400°C (Kobchenko et al., 2011; Panahi et al., 2013). The
103 samples, 25 mm diameter and height, were cored perpendicularly to bedding. The kerogen is
104 organized into small elongated patches, 10-200 micrometers long and 2-5 micrometers thick,
105 spread along preferential beds in the shale. The microstructure of the rock was imaged before
106 heating using high resolution X-ray microtomography at beamline ID19 at the European
107 Synchrotron Radiation Facility (Grenoble, France), at a voxel size of 0.16 micrometer, allowing
108 identification of the 3D geometry of kerogen patches (Figure 1).

109 A steel sample holder was custom-made to contain the sample and simulated a moderate
110 confinement. Some holes were drilled into the holder to enable the fluids released during
111 experiments to escape. A wave spring was used to apply an axial load to the samples, while the
112 vessel was pressurized at 10 bars with nitrogen gas. The sample was not jacketed and a small
113 differential state of stress was applied to the samples by the wave spring that applied a force on
114 the top surface of the sample, equivalent to an axial stress of 12 bars. The present experiments
115 did not reproduce the whole maturation process at conditions of several kilometers depth in
116 sedimentary basins. Rather, the main motivation was to show that the presence of a small
117 differential stress can explain the formation of a connected 3D network of microfractures. We
118 observed that the organic matter transformed into oil, as observed by some hydrocarbon stains
119 released in the pressure vessel and around the rock samples after the experiments. Moreover,
120 visible fractures could be seen on the outer surface of each sample, which were imaged in 3D

121 using a laboratory X-ray microtomograph with a voxel size of 11 micrometers. The 3D volumes
122 were processed using the software AvizoFire™ to visualize the fractures.

123 **2. 2 Numerical simulation of shale maturation**

124 Numerical modeling was used to evaluate the possible mechanisms of kerogen maturation-
125 induced microfracturing. In particular, the discrete element method (DEM) was chosen because
126 of its capability to simulate the propagation of fractures within a rock matrix containing pre-
127 existing heterogeneities such as bedding and varying kerogen concentration along laminations
128 (Scholtès and Donzé, 2012). For instance, this method has already been used for the analysis of
129 rock failure mechanisms involving wing crack propagation (Duriez et al., 2016), fractures
130 coalescence (Scholtès and Donzé, 2012) or even hydrofracture propagation (Papachristos et al.,
131 2016).

132 The simulations were performed with the YADE Open DEM platform (Kozicki and Donzé,
133 2008, Kozicki and Donzé, 2009; Smilauer et al., 2015), where the solid phase is represented by
134 a discrete element packing whose respective motion is ruled by Newton's second law and the
135 fluid flow is simulated using a finite volume method (Catalano et al., 2014). Regarding the
136 mechanical behavior of the model, each interaction force linking the discrete elements obeys
137 an elastic-brittle behavior in both normal and tangential directions. Under stress or strain
138 loading, the bonds can break by either tensile or shear failure mechanism, following a modified
139 Mohr-Coulomb criterion with a tension cut-off (for details, see Scholtès and Donzé, 2013). The
140 fluid flows through an interconnected pore network located in between the discrete elements
141 (dual space). The DEM and finite volume methods are fully coupled in the sense that any
142 deformation of the solid phase affects the fluid flow and, conversely, any variation in pore
143 pressure induces deformation of the medium (Papachristos et al., 2016). The local interporal
144 fluid conductance k is formulated in order to capture the high permeability contrast between the
145 fractures and the intact rock matrix (Figure 2a). The conductance of the throats connecting the
146 pores located in the intact rock matrix is computed as proposed by Chareyre (2012). While
147 fractures form, i.e. when broken bonds are identified in the model, the corresponding pore throat
148 is replaced by a parallel plate model and the flow governed by the cubic law. k is then computed
149 as a function of the fracture aperture which is updated at each time step of the simulation
150 (Papachristos et al., 2016).

151 We choose here to model a tight rock with petrophysics parameters typical of a shale located at
152 5 km depth (Sone and Zoback, 2013), and a fluid with properties (viscosity and bulk modulus)
153 similar to that of water. Table 1 shows the values of the parameters used to model the problem
154 (Abousleiman et al., 2008). We consider a 26 mm size cubic sample, represented by a dense
155 packing constituted of 10000 discrete elements (Figure 2b). The system is isothermal and heat
156 exchanges are not considered.

157 The microstructure of the numerical samples takes into account two observations (Figure 1).
158 Some layers at the millimeter scale are kerogen-rich, and the kerogen is organized into
159 ellipsoidal patches, i.e. a set of pre-existing heterogeneities considered as initial fractures in the
160 model. As a result, we designed a synthetic shale sample that contains layers and ellipsoidal
161 patches of organic matter (Figure 2c). The number of kerogen patches (1, 2, or 13), their
162 persistences (parameter $p=d/D$ in Figure 3), and relative positions in the kerogen-rich layers
163 are varied. Here, the persistence p is a dimensionless geometric parameter that represents the
164 ratio between the diameter d of kerogen patches and the distance D between the centers of two
165 neighboring patches. To simulate kerogen maturation, the fluid pressure is increased
166 progressively in each pre-existing kerogen patches by imposing a constant flow rate at their
167 centres. As a result of the pressure buildup, fracturing occurs along the kerogen-matrix interface
168 (at the tips of the kerogen patches), driving the fluid to propagate into the low permeable rock
169 matrix before escaping freely outside the sample (a fluid pressure of 0 Pa is imposed at its
170 boundaries). In addition, the sample can be confined under isostatic external stress with $\sigma_h =$
171 $\sigma_H = \sigma_v = 80$ MPa or under differential stress state with $\sigma_h = \sigma_H = 80$ MPa, while σ_v can be
172 varied between 90 and 110 MPa. Here, $\sigma_h = \sigma_H$ are the two main horizontal stresses and σ_v is
173 the vertical stress applied on the sample's boundaries (Figure 2b).

174 In the present study, the experiments are used to illustrate the physical process of fluid expulsion
175 during kerogen maturation and the numerical simulations are performed to explore a range of
176 parameters rather than reproduce directly the experiments. For this reason the choice of
177 geometrical parameters for the simulations is a compromise between comparing simulation
178 results with the specific Green River shale used in the experiments and providing a physical
179 understanding of the control parameters of fluid expulsion during kerogen maturation. In the
180 simulations, the size of the sample is centimeter scale (Figure 3), as in the experiments (Figure
181 4a), and the ratio between the kerogen patch diameter and the distance between the centers of
182 two kerogen patches, which is referred to as the persistence, is similar as well. However, to be

183 able to characterize the effect of individual kerogen patches, we have chosen dimensions of
184 kerogen patches larger in the numerical simulations (several millimeters) than in the natural
185 Green River shale (several hundred micrometers).

186 Simulations were performed by varying from one, two, up to thirteen the number of kerogen
187 patches as well as their size in the numerical sample. With one patch, the propagation of a single
188 fracture can be modelled. With two kerogen patches, local stress and progressive failure
189 interactions are studied when both fractures propagate simultaneously. With thirteen initial
190 kerogen patches, orientation and connectivity trends occurring during microfracturing can be
191 observed. This geometry is used to upscale from single kerogen patch to the microfracturing of
192 the whole rock, taking into account the interaction process between several fractures, which has
193 been neglected in previous works (e.g. Lash and Engelder, 2005; Zhang et al. 2008). In the
194 simulations with one or two kerogen patches, the diameter d of the patch was set to a value of
195 6 mm. The horizontal offset L between the patches was varied between 0 and ± 2 mm for
196 simulations with two patches.

197 In the simulations with thirteen kerogen sources, the patches are located in three different layers
198 with 4, 5 and 4 patches located at 7, 13, and 19 mm from the bottom in the vertical direction,
199 respectively (Figure 3). In addition, the patch diameter d was varied between 1, 4, 6, and 7 mm,
200 corresponding to a persistence p of 0.12, 0.47, 0.71 and 0.83, respectively, p being defined by
201 $p = d / D$, with $D = 8.5$ mm, the distance between the center of the kerogen patches. The value
202 $d = 6$ mm was chosen such that the total surface area of the kerogen in the intermediate layer is
203 equal to 20% of the section area of the kerogen-rich bed in that sample. The present simulations
204 could be rescaled for smaller size kerogen patches and smaller rock volumes, as those observed
205 in the tomography data of the Green River shale samples where d and D are ten to fifty times
206 smaller, whereas the persistence p is the same as in the numerical simulations.

207 **3. Results**

208 **3.1 Experiments of shale maturation**

209 The maturation of Green River shale samples to temperatures up to 390°C was previously
210 studied time-lapse during heating (Kobchenko et al., 2011; Panahi et al., 2013) and it was shown
211 that fractures developed parallel to bedding in absence of confining stress and differential stress.
212 Here, a small axial differential stress of 12 bars is applied to the sample, and under the effect of

213 heating hydrocarbon is produced, as suggested by the presence of stains of oil on the sample
214 after maturation (Figure 4a). Using X-ray microtomography imaging, the microstructure of the
215 fractured shale becomes clearly visible. Most of the microfractures are horizontal (Figure 4c-d)
216 and parallel to the bedding. They have formed presumably by the lateral propagation of
217 fractures initiating off kerogen patches (Figure 4b), due to local overpressure build-up during
218 kerogen maturation. Interestingly, several fractures are also oriented vertically. The maturation
219 process under a small differential stress allows the formation of a fracture network that
220 percolates in three-dimensions across the whole volume, allowing the fluid to freely escape
221 (Figure 4c-e). The main difference with previous studies for which no differential was applied
222 (Kobchenko et al., 2011; Panahi et al., 2013) is that here both horizontal and vertical
223 microfractures could develop, creating a connected network in three dimensions. To
224 summarize, axial differential stress favors vertical growth whereas bedding anisotropy favors
225 horizontal growth.

226 3.2 Numerical simulations

227 Under an increase of local pressure in the kerogen patches, fluid escapes by breaking
228 interparticle cohesive bonds and thus creating damage (i.e. microfractures) inside the rock
229 matrix. To quantify this damage and the associated fluid migration, we calculate the value of
230 the parameter P_{32} that represents the intensity of the fractures, i.e. the total surface of the
231 fractures divided by the total volume of the numerical sample (Papachristos et al., 2016) and
232 that is defined as:

$$233 \quad P_{32} = \frac{\sum A_i}{V} \quad (1)$$

234 with A_i the surface area of the i^{th} microfracture, and V the initial volume of the sample.

235 The orientation of hydraulically induced microfractures is quantified by defining the dip angle
236 θ , i.e. the angle between the vector normal to the microfracture surface and the vertical axis of
237 the sample. If only horizontal fractures are present, the angles θ cluster around 0° ; whereas in
238 case of vertical fractures, θ reaches 90° . Finally, the vertical interconnectivity of the
239 microfractures is expressed using a fracture layer ratio of damage in kerogen-free and kerogen-
240 rich layers, which is characterized through the parameter K defined as:

241
$$K = \frac{NK}{WK} \tag{2}$$

242 with NK the quantity of microfractures in kerogen-free layers (*No Kerogen*), and WK the
243 quantity of microfractures in kerogen-rich layers (*With Kerogen*) (Figure 5). NK and WK
244 represent the values of P_{32} (Equation 1) in both layers. In the following sections, the main results
245 of the simulations are presented.

246 3.2.1 Damage around a single kerogen patch

247 Here, we consider a patch of kerogen with a diameter $d = 6$ mm, located at the center of the
248 sample, where fluid pressure is increased with time. Four simulations were performed where
249 the vertical compressive stress σ_v was varied between 80 and 110 MPa, while the horizontal
250 stresses were maintained constant and equal to 80 MPa. A vertical section is made through the
251 middle of the numerical sample (Figure 6), where the red discs represent the newly created
252 microfractures propagating from the initial horizontal kerogen patch and where fluid migration
253 is highlighted by the dark cells of the finite volume mesh. Microfractures nucleate at the tip of
254 the initial kerogen patch, before propagating away. For a hydrostatic stress state loading, the
255 resulting fracture composed of the connected microfractures stays in the plane of the source
256 fracture, as observed in experiments (Kobchenko et al., 2011). A different behavior can be
257 observed for a differential stress state of 20 MPa where the microfractures tend to rotate towards
258 the direction of maximum compressive stress σ_v and grow initially at an angle of 30° with the
259 vertical direction. Away from the initial source fracture, these microfractures tend to become
260 aligned with the vertical direction. As a consequence, fluid also tends to migrate along the
261 direction of maximum stress where fractures open under the application of a differential stress
262 as usually found in sedimentary basin. Moreover, the amount of microfracturing measured by
263 the parameter P_{32} (Figure 7b) shows a slight linear decrease as the vertical stress increases,
264 whereas the ratio of microfractures in kerogen-free compared to kerogen-rich layers increases
265 with increasing vertical stress (Figure 7a). The decrease of P_{32} with increasing vertical stress is
266 due to the fact that, at the onset of microfracturing, a higher overpressure in the kerogen patch
267 is necessary to fracture the matrix around when the external stress is increased. Moreover,
268 increasing the differential stress enhances the localization of the deformation into a narrower
269 damage zone, whose propagation path follows more directly the direction of the main
270 compressive stress. The increase of K , which is about one order of magnitude, shows that,
271 besides the re-alignment of the microfractures with the maximum stress, an important spatial

272 reorganization of the microfractures network takes place under a state of differential stress,
273 which enhances the interlayer connectivity.

274 **3.2.2 Damage around two kerogen patches**

275 In these simulations, one kerogen patch is located 10 mm above the bottom of the sample and
276 the second patch at 16 mm. The relative position, i.e., the horizontal distance L between the
277 kerogen patches is varied between $-2r$, $-r$, 0 , r and $2r$, where r is the radius of the patch equal
278 to 3 mm in these simulations, and the minus sign represents the vertical superposition of the
279 initial fractures (Figure 8). The vertical stress σ_v is varied between 80 and 100 MPa.

280 The damage due to kerogen maturation and fluid migration evolves spatially under the influence
281 of both the imposed external stress and the local stress field generated by the pressure increase
282 in each kerogen patch, allowing stress interactions depending on the relative position of the two
283 patches (Figure 8). There is a clear effect on damage pattern from both parameters. When the
284 two kerogen patches tips are vertically aligned (Figures 8a, 8c), the stress interaction is at its
285 maximum (Jiang et al., 1991) and contributes to increase the vertical connectivity by a
286 coalescence process. Note that, in the case of vertically aligned kerogen patches (Figures 8d),
287 the dilatancy due to the over-pressurized fluid also increases the compressive stress in between
288 the patches, leading to a strong fracture interaction (Papachristos et al., 2016). When the two
289 kerogen patches are separated by too large a distance ($r > 2$ mm), no stress interaction could be
290 seen, limiting therefore the inter-layer connectivity (Figure 9).

291 The increase of the vertical differential stress enhances the rotation of microfractures toward
292 the direction of the maximum principal stress, allowing a faster coalescence between the
293 damage zones (Figure 8c). This is also clearly measured from the total surface area of the
294 microfractures (P_{32}), which is greater when the vertical compressive stress is larger. We also
295 show below that this parameter P_{32} increases even more with increasing differential stress
296 when more than two kerogen patches are present, demonstrating the importance of local
297 interactions between several sources of overpressure.

298 **3.2.3 Damage with thirteen kerogen patches**

299 In these simulations, a larger number of kerogen patches (thirteen) are inserted into the shale
300 model. This geometry is closer to what can be observed in a natural sample. The patches are
301 located in three layers (Figure 3). The patch diameters are varied between 1-7 mm,

302 corresponding to a persistence p in the range 0.12-0.83. The external vertical compressive stress
303 is varied in the range 80-110 MPa, for constant horizontal stresses equal to 80 MPa.

304 The influence of the vertical stress on microfractures development is presented in [Figure 10](#)
305 where a vertical slice is made through the center of the volume as illustrated on [Figure 3](#). Similar
306 to the results shown in [Figures 6](#) and [8](#) for a smaller number of kerogen patches, the local
307 maximum stress ([Figure 10a](#)) tends to align with the maximum applied stress direction ([Figure](#)
308 [10b](#)). According to this reorientation, it can be observed once again that the distribution of
309 generated microfractures is strongly affected by the existence of the differential stress. A
310 systematic analysis of the orientation of the newly formed microfractures is shown on [Figure](#)
311 [11](#). There is a clear effect of the imposed external stress: the microfractures tend to rotate
312 preferentially towards the vertical axis as σ_v increases. For intermediate values of σ_v , the rose
313 diagrams show that the microfractures are oriented in all directions, favoring a 3D network. At
314 low differential stress most of them are horizontal (the initial kerogen microstructure
315 dominates), whereas at high differential stress most of them are vertical (the external loading
316 dominates).

317 The effect of persistence p (see [Figure 3](#)) on the intensity and spatial distribution of the
318 microfractures is presented in [Figure 12](#). The evolution of the relative value of the ratio K shows
319 a strong non-linearity as the differential stress becomes important, as can be expected during
320 an extensive tectonic episode ([Figure 12a](#)). In the case of highly persistent kerogen patches ($p >$
321 0.71 in [Figure 12b](#)), the amount of new microfractures does not need to massively increase to
322 connect the different patches, and the microfracture intensity values remain low. However, it
323 can be seen that the increase of the differential stress remains of secondary effect on the
324 evolution of the microfracture intensity ([Figure 12b](#)).

325 **4. Discussion**

326 **4.1 Microfractures in shales**

327 Several studies have been performed to address microfracturing in tight rocks because natural
328 fractures in shales play a role in controlling cap rock integrity. They focused on technologies
329 related to underground nuclear waste disposal and, more recently, geological storage of CO₂
330 (e.g. [Bolton et al., 2000](#); [Yang and Aplin, 2007](#); [Sarout and Guéguen, 2008](#); [Ababou et al.,](#)
331 [2011](#); [Skurtveit et al., 2012](#); [Ghayaza et al., 2013](#)). Open microfractures from the nanometer to

332 micrometer scale affect the physical properties of rocks, such as compressibility, strength,
333 elastic wave velocities, and permeability (Kranz, 1983). The fluid transport properties of low-
334 permeability rocks are primarily controlled by the structure of available flow pathways (Keller
335 et al., 2011) such as microfractures, the rock matrix having much lower permeability and high
336 capillary entry pressure. Microfractures also control the long-term sealing capacities of cap-
337 rocks and the expulsion of hydrocarbons during primary migration. In this case, the fluid which
338 escapes due to mechanical compaction or generation of hydrocarbons is determined by the
339 width and spacing of the fractures. As the effective stress in the cap-rock changes, because of
340 increasing fluid pressure in the underlying reservoir, fractures may be created and/or
341 reactivated, and they may close when the fluid pressure in the reservoir decreases because of
342 loss of fluid through the fractures. It is particularly important to understand and characterize
343 these properties in deep reservoirs, for which exploration and production boreholes are
344 particularly costly.

345 Several processes contribute to microfracture formation in borehole cores and in outcrop
346 samples (Vernik 1994; Dewhurst et al., 2011). Some of these occur during sample recovery or
347 exhumation and unloading, while others occur naturally at depth. Actually, two types of
348 microfracture orientations can be identified in shales. The first type is oriented parallel to the
349 bedding, along planes of weakness, and the second type, oriented at high angles relative to the
350 first, may intersect the first to form a 3D network that greatly increases the permeability and
351 reduces the capillary entry pressure in the vertical direction (Breyer, 2012; Padin et al., 2014;
352 Kalani et al., 2015). The existence of these two types of microfractures is a necessary, but not
353 sufficient, condition for the formation of a percolating microfracture network at the decimeter
354 to meter scale. In the present study, we characterize how hydrocarbon maturation can lead to
355 the formation of a percolating microfracture by varying both the external state of differential
356 stress and the amount and geometry of initial kerogen patches in shales.

357 **4.2 Microfracture formation by kerogen maturation**

358 Microfracturing in shales involves several steps from the nucleation of microfractures, their
359 propagation, and their final arrest either as a dead end or as a connection to another fracture or
360 a discontinuity such as sedimentary bedding (Chandler et al., 2013). The process of shale
361 maturation and primary migration was reproduced experimentally in recent studies. In a series
362 of laboratory experiments performed on immature shales, the fracturing process was visualized
363 using either scanning electron microscopy (Allan et al., 2014) or time-lapse synchrotron X-ray

364 microtomography (Kobchenko et al., 2011; Panahi et al., 2013; Saif et al., 2016). These
365 experiments show that microfractures initiate in the kerogen patches, where fluids are produced
366 and fluid pressure builds up, and then propagate preferentially along the direction of layering.
367 However, neither confining pressure nor differential stress was applied to these samples during
368 the experiments, and formation of a connected 3D fracture network was not observed.
369 Conversely, the application of a small differential stress is a necessary condition for the
370 formation of vertically oriented microfractures (Figure 4).

371 If fluid is generated within or injected into a spherical cavity in a (hypothetical) homogeneous
372 rock, fracturing is expected to occur in the plane perpendicular to the direction of the
373 (horizontal) far field least principal compressive stress, when the fluid pressure becomes large
374 enough. However, fluid producing kerogen and clay mineral flakes, oriented preferentially
375 along the bedding plane, constitute weak microstructures that act as pre-existing microfractures
376 that propagate along the bedding direction as they are inflated by progressive fluid production.
377 This happens during kerogen maturation that leads to an overall volume increase on the order
378 of 10-20% and a local pressure that may be high enough to fracture source rocks (Pelet and
379 Tissot, 1971; Vernik, 1994; Hunt, 1990; Capuano, 1993; Vernik, 1994; Jin et al., 2010). The
380 anisotropic rock strength, also a consequence of the orientation of strongly anisometric kerogen
381 flakes and inorganic mineral grains, also favors fracture growth along the bedding plane (e.g.
382 Keller et al. 2011; Harrington and Horseman, 1999). Some microfractures may nucleate along
383 directions that are inclined at large angles relative to the bedding plane, and fractures that are
384 propagating in the direction of the bedding plane may be diverted by heterogeneity. For
385 example, while high aspect ratio kerogen flakes, which are typically oriented along the bedding
386 plane, favor horizontal microfractures, low aspect ratio flakes favor vertical fractures (Ozkaya,
387 1998; Lash and Engelder, 2005). Although relatively few in number, vertical growth of these
388 fractures is favored by the far field stress, and they may become large enough to connect many
389 horizontal microfractures leading to the formation of a 3D fracture network that enables fluid
390 flow on the scale of a sedimentary layer, which would further facilitate hydrocarbon primary
391 migration (Fan et al., 2012). This effect of a small differential stress on fracture network growth
392 in 3D is shown both in our experiments (Figure 4) and in the numerical simulations (Figures 10
393 and 11).

394 **4.3 Dynamics of microfractures during primary migration**

395 Analogue experiments have been performed using transparent brittle hydrogels that enable
396 optical characterization of the fracturing dynamics driven by internal gas production (Bons and
397 van Milligen, 2001; Kobchenko et al., 2013, 2014; Zanella et al., 2014). In these systems, CO₂-
398 producing yeast was mixed into a brittle solid (i. e. the gel). With gas production, microfractures
399 nucleate in the elastic solid and then propagate, leading to the formation of a well-developed
400 fracture network that facilitates gas expulsion. Several results relevant to the development of
401 conceptual models for shale maturation and fluid expulsion emerged from these experiments.
402 Firstly, the fracture network has geometrical and topological properties that are intermediate
403 between those of two end-member drainage networks found in nature, namely river systems
404 and hierarchical fracture networks (Kobchenko et al., 2013). Secondly, these experiments show
405 that gas expulsion and fracture opening and closing are intermittent, and that the fractures close
406 once all the gas has been produced in the solid and escaped from it. Moreover, the dynamics of
407 individual fracture opening and closing are rather complex, with a power-law gas volume
408 fluctuation spectrum, due to the long-range elastic interactions in the solid (Bons and van
409 Milligen, 2001, Kobchenko et al., 2014). These experiments show that the microfracturing
410 process is controlled by several parameters, including the amount of fluid produced during
411 maturation, the kinetics of maturation, the permeability and elastic parameters of the solid and
412 the thickness of the elastic layer in which fluids are produced. These experiments also show
413 that once the fractures formed, they may close completely when the produced fluid has escaped,
414 leaving behind well-defined low-cohesion interfaces, which may heal or cement over time.
415 Making an analogy with shales, microfractures therefore appear to form during maturation and
416 then close. When closed, their transport properties are similar to those of the shale matrix or
417 depend on local cementation. However, if the fluid pressure increases, they can be preferentially
418 reopened, providing pathways for fluid transport.

419 Our results show that the state of stress in shales during maturation and the initial geometry of
420 the kerogen patches control the final geometry of the microfractures produced. Importantly, the
421 presence of a differential stress, even small, is enough to produce a network of fractures
422 percolating in 3D. At zero differential stress, the final geometry is controlled by the layers where
423 kerogen is concentrated and microfractures are mainly bed parallel. Under the effect of a
424 moderate differential stress, microfractures development is controlled by the external loading
425 and initial kerogen patches distribution with the microfractures being oriented both horizontally
426 and along the direction of the main compressive stress.

427 To summarize, in organic-rich immature shales, patches of kerogen are disseminated in the
428 matrix along preferential beds and are oriented parallel to sedimentary layering. With
429 maturation, the organic matter decomposes, increases locally the fluid pressure, and produces
430 oil and gas that escape through the formation of horizontal and vertical microfractures. A
431 fracture network forms when horizontal and vertical microfractures cross-cut in 3D and create
432 a percolating flow path, allowing primary migration (Figure 13). The initial geometry of the
433 patches, their density in the matrix, and the external stress control the final geometry of the
434 fracture network. The local stresses due to fluid overpressure interact with the external stresses
435 applied on the medium. Depending on these interactions, the microfractures may be oriented
436 mainly parallel to the bedding (low differential stress, large kerogen patches), perpendicular to
437 it (high vertical stress) or form a 3D network that percolates through the entire volume.

438 **5. Conclusion**

439 The influence of external and internal parameters on the microfracturing of immature shales is
440 investigated here through a coupled experimental and numerical approach. Green River shales
441 were heated until the organic matter they contain matured and produced hydrocarbon that
442 escaped by fracturing the matrix. In the presence of a small differential stress, both bed-parallel
443 and bed-perpendicular fractures form, creating a percolating network in three dimensions.
444 Discrete element numerical simulations show that, at constant temperature, the controlling
445 parameters are the initial geometry of the kerogen patches and the state of external stress. The
446 main results are:

- 447 1) Due to their preferential orientation, kerogen patches tend to favor initial fracturing in
448 directions parallel to bedding;
- 449 2) In the presence of a differential stress, with the vertical compressive stress larger than
450 the horizontal stresses, vertical fractures can develop.
- 451 3) The density of microfractures depends on initial kerogen composition and external
452 stress.
- 453 4) The conditions under which a percolating network of fractures is formed, allowing fluid
454 escape and primary migration are identified and it is shown that the presence of a differential
455 stress is necessary, and that an initial configuration where kerogen patches are organized in
456 several layers is necessary to connect vertically microfractures and allow fluid expulsion.

457

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462 and Jacques Desrues at the Laboratoire 3S-R, UMR 5521 CNRS, Univ. Grenoble Alpes for the
463 laboratory tomograph acquisitions (data in Figures 4 and 13).

464

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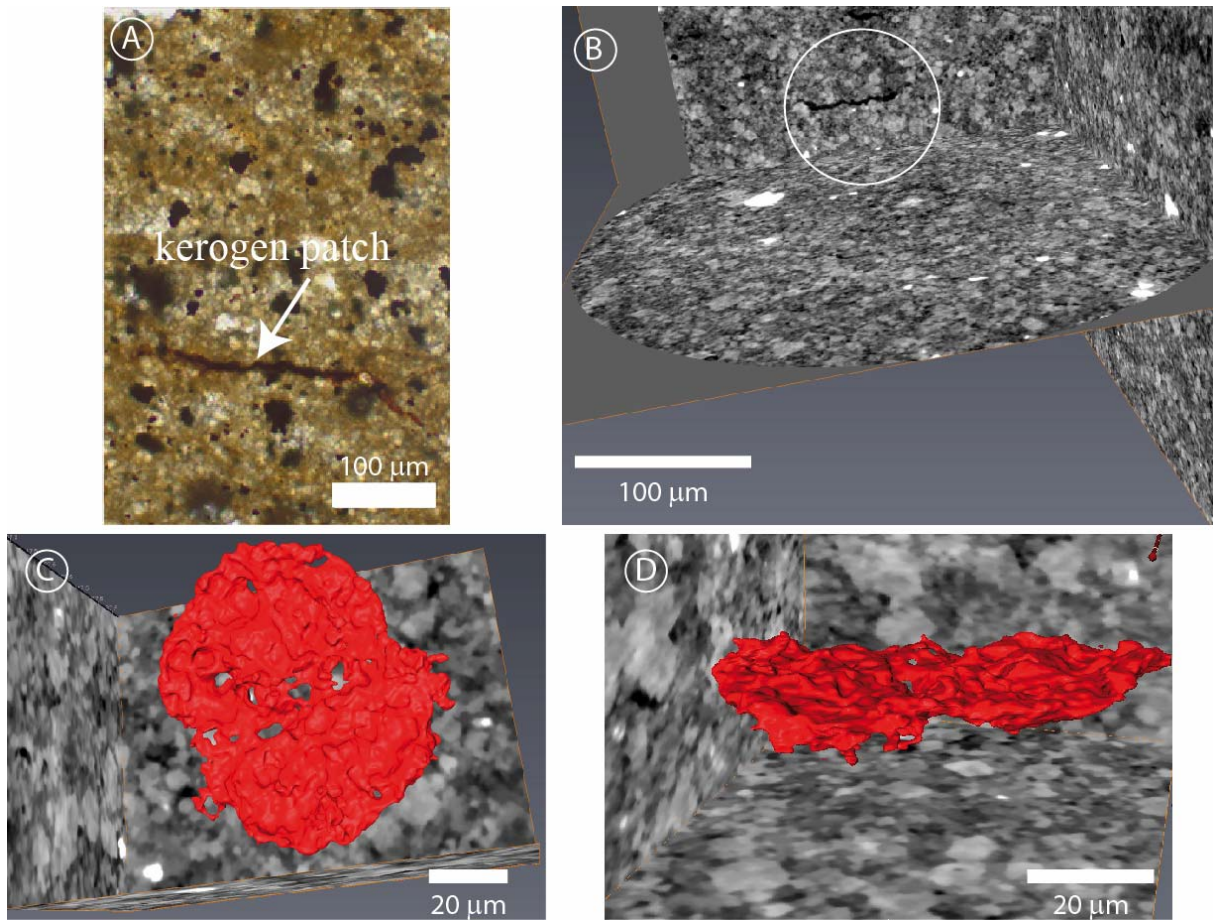
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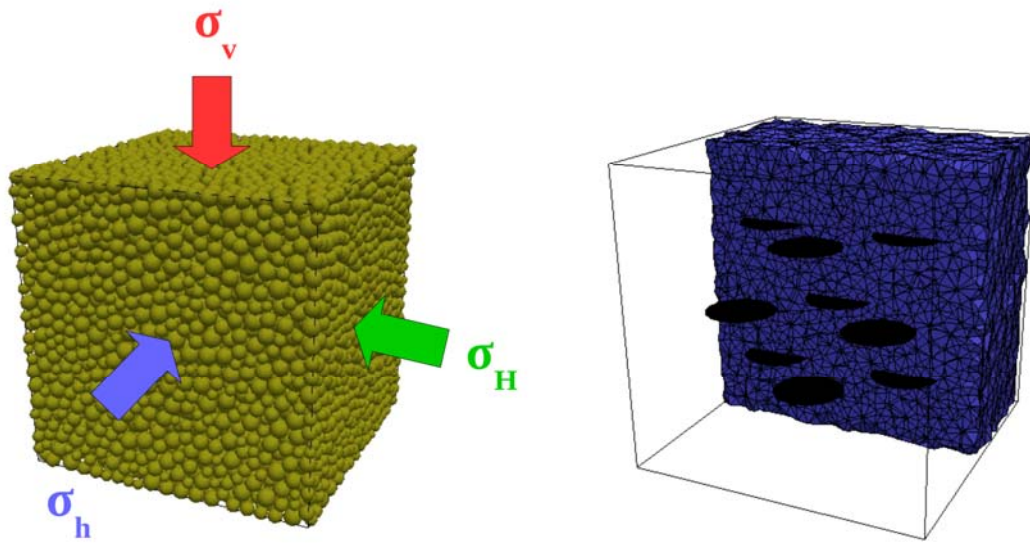
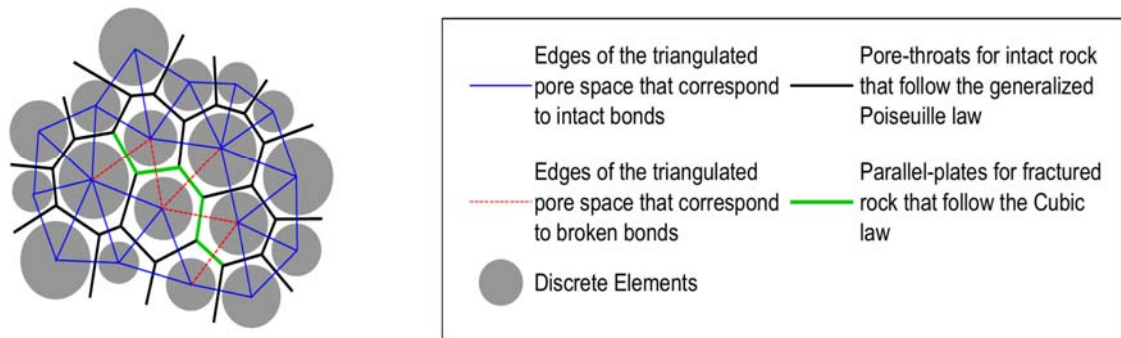
621 Figure 1: Imaging of kerogen in a Green River shale sample. A) Optical microscopy showing
622 a kerogen patch. B-D) X-ray microtomography imaging of a Green River shale sample at a
623 voxel size of 0.16 micron showing the microstructure of the shale where the various gray scale
624 levels underline the individual grains (for example pyrite minerals appear in white). A kerogen
625 patch is parallel to bedding (white circle in B). C-D) Zooms on a patch of kerogen which forms
626 an ellipsoid, 70 micrometers wide and 2-4 micrometers height. The outer surface of the bed
627 parallel kerogen patch is colored in red.

628

629 Table 1: Properties of the synthetic shale rock and fluid used in the numerical simulations. UCS:
 630 Uniaxial Compressive Strength. UTS: Uniaxial Tensile Strength.

Shale model		Fluid	
Density	2500 kg/m ³	Bulk	2.2E9 Pa
Young's modulus	26x10 ⁹ Pa	Viscosity	10 ⁻³ Pa s
Poisson's ratio	0.25	Flow rate	10 ⁻⁶ m ³ /s
UTS	3 MPa		
UCS	25 MPa		
Permeability	10 ⁻²³ m ²		

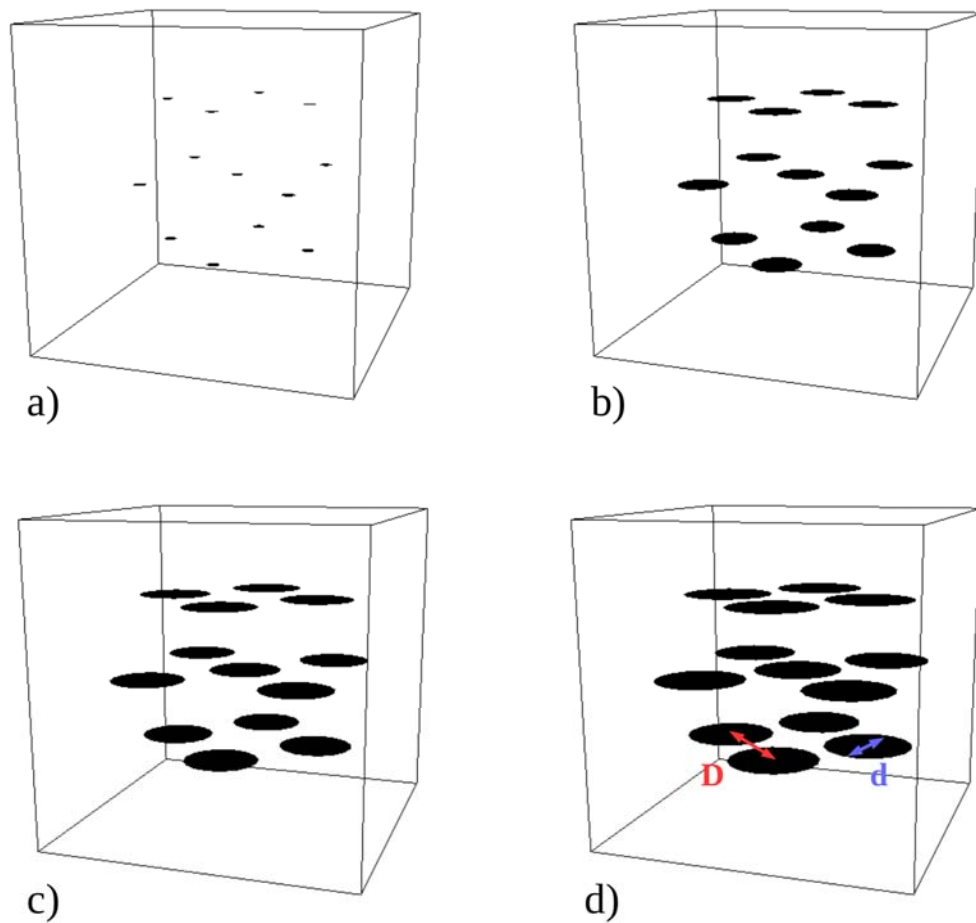
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633 Figure 2: a) Principles of the numerical model illustrated by a 2D slice sketch. b) 3D view of
 634 the shale rock volume with discrete elements and c) the associated finite volume mesh for the
 635 fluid with the patches of kerogen represented as black ellipsoids.

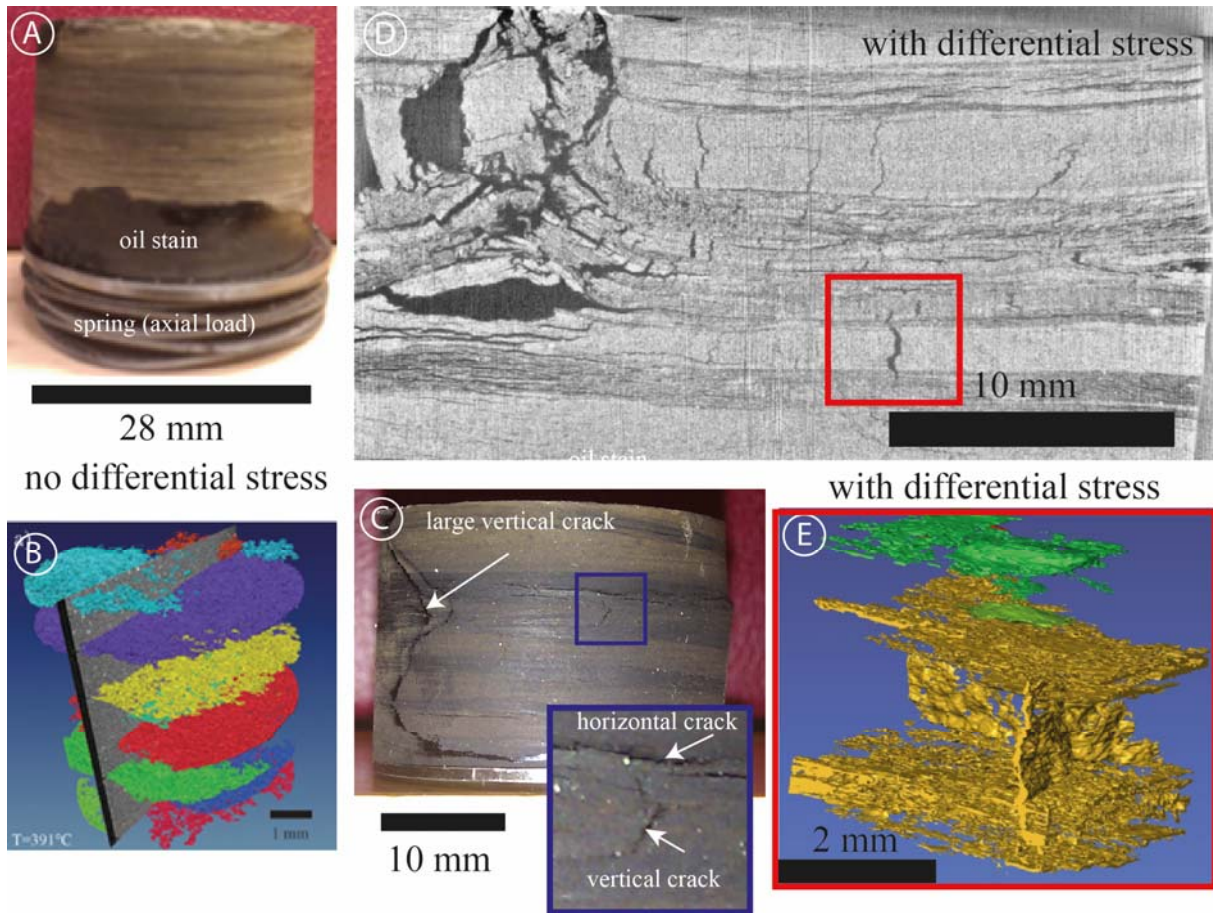
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638 Figure 3: Side-view of the inside of the shale rock that contains patches of kerogen represented
 639 as ellipsoids (see Figure 1c-d). The number of patches is initially fixed (here 13) and the
 640 persistence $p = d / D$ is varied, where d is the size of each patch and D is the distance between
 641 them. Taking $D = 8.5$ mm, different persistence values can be obtained with a) $p = 0.12$ ($d = 1$
 642 mm), b) $p = 0.47$ ($d = 3$ mm), and c) $p = 0.71$ ($d = 8.5$ mm), and d) $p = 0.83$ ($d = 10$ mm). In the
 643 numerical model the persistence is similar to that in the Green River Shale sample, whereas d
 644 and D are ten to hundred times smaller in the natural sample.

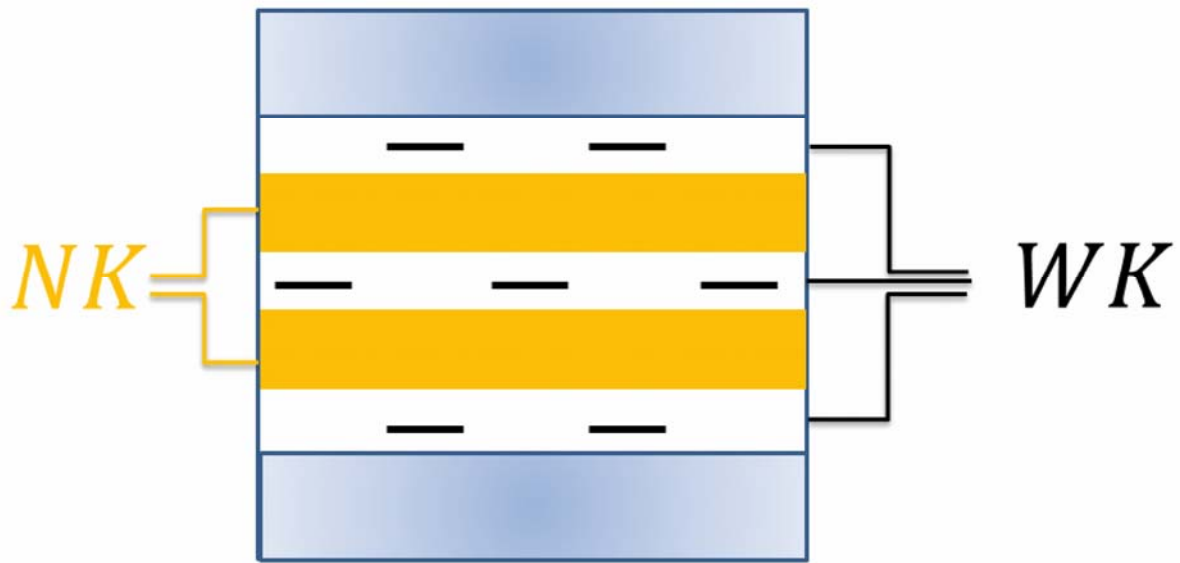
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647 Figure 4: Shale sample after heating at 390°C for 24 hours. A) Sample core sample with the
 648 wave spring (at the bottom) that imposed a small differential stress inside the pressure vessel.
 649 A stain of hydrocarbon (dark) is visible after maturation. B) Microtomography imaging of
 650 fractures in a sample heated at atmospheric pressure (adapted from [Kobchenko et al., 2011](#)). C-
 651 D) 2D slices from 3D X-ray micromotography data of a sample heated under differential stress
 652 after maturation. The initial horizontal bedding and the horizontal and vertical fractures
 653 produced by kerogen maturation and hydrocarbon maturation can be seen. E) 3D view of the
 654 fracture network with connecting horizontal and vertical fractures.

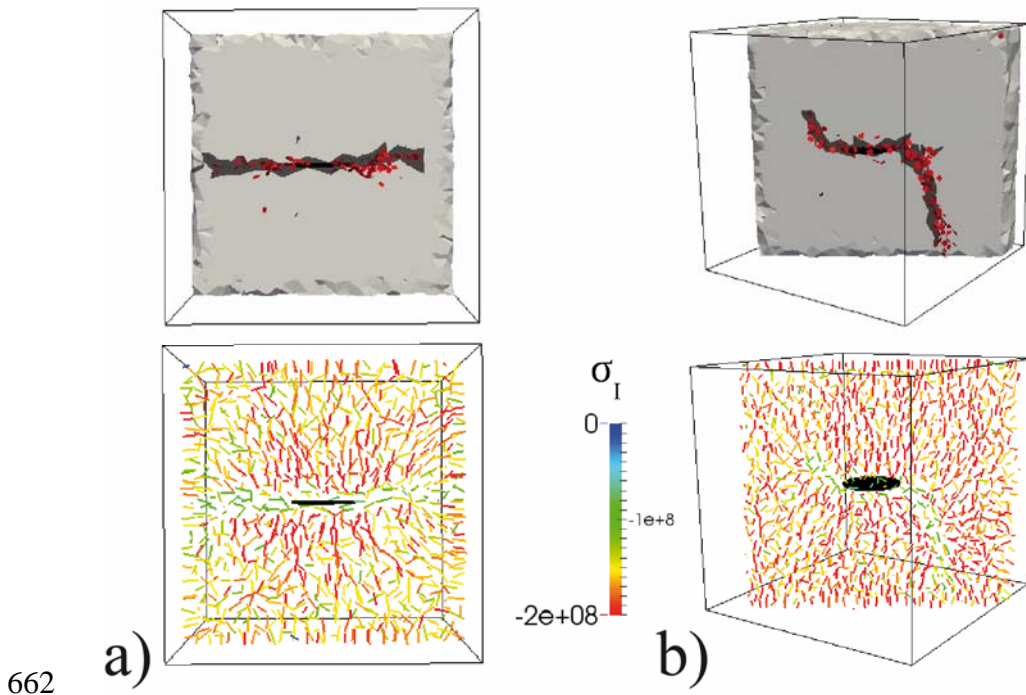
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657 Figure 5: Definition of the parameters NK (kerogen-free layers: *No Kerogen*) and WK
 658 (kerogen-rich layers: *With Kerogen*). The surface area of newly created microfractures
 659 (parameter P32, see Equation 1) is calculated in kerogen-free and kerogen-rich layers,
 660 respectively, and the ratio between these two numbers is called K (see Equation 2).

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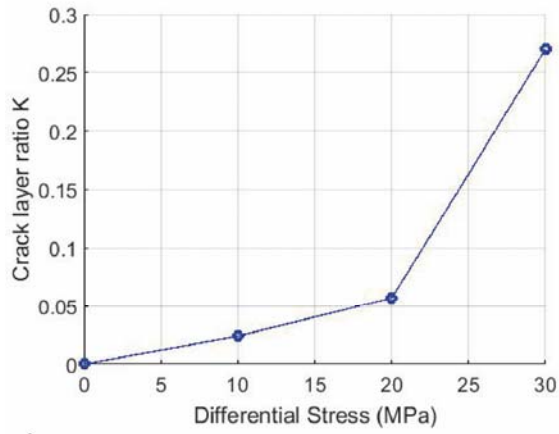
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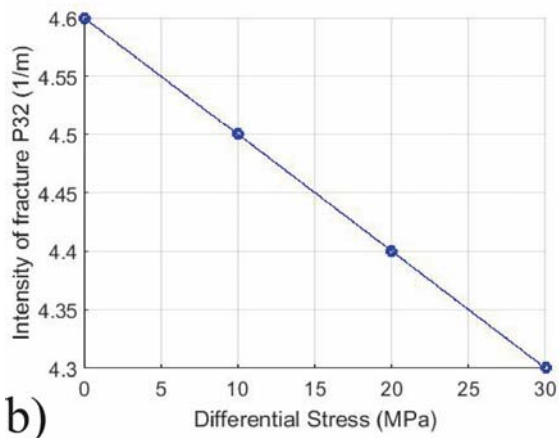
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Figure 6: Left side: Slice in the middle of the sample showing microfractures (red discs) and fluid migration (dark gray cells) around a single horizontal kerogen patch for (a) the hydrostatic case with $\sigma_v = 80$ MPa and (b) a differential stress of 20 MPa with $\sigma_v = 100$ MPa. On the right side, the direction and intensity of local maximum principal stresses σ_1 (Pa) are represented as thin lines colored as a function of their intensity for each case.



a)

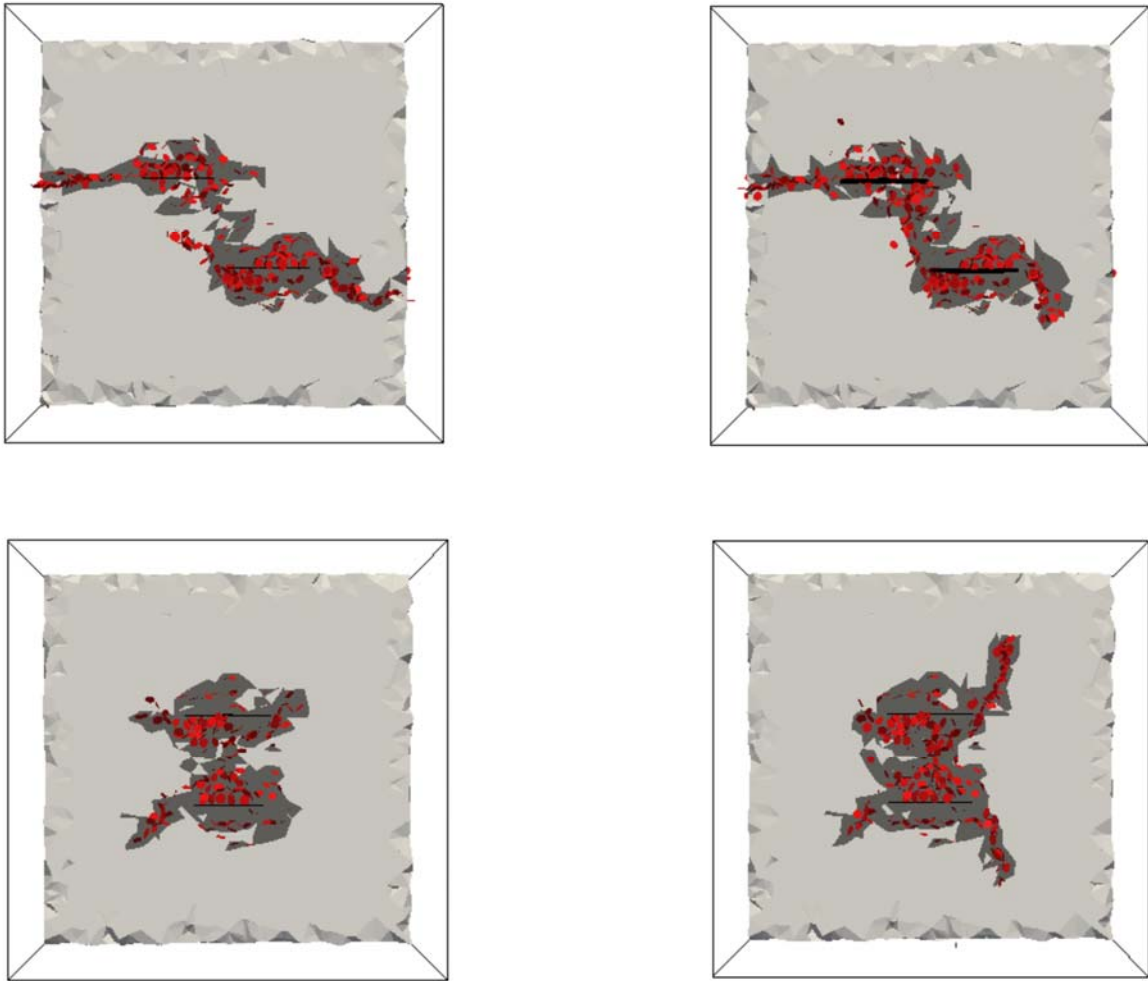


b)

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670 Figure 7: a) Evolution of the ratio K of microfractures in kerogen-free compared to kerogen-
 671 rich layers. b) Intensity of fracturing (parameter P32, see Equation 1) versus differential stress.

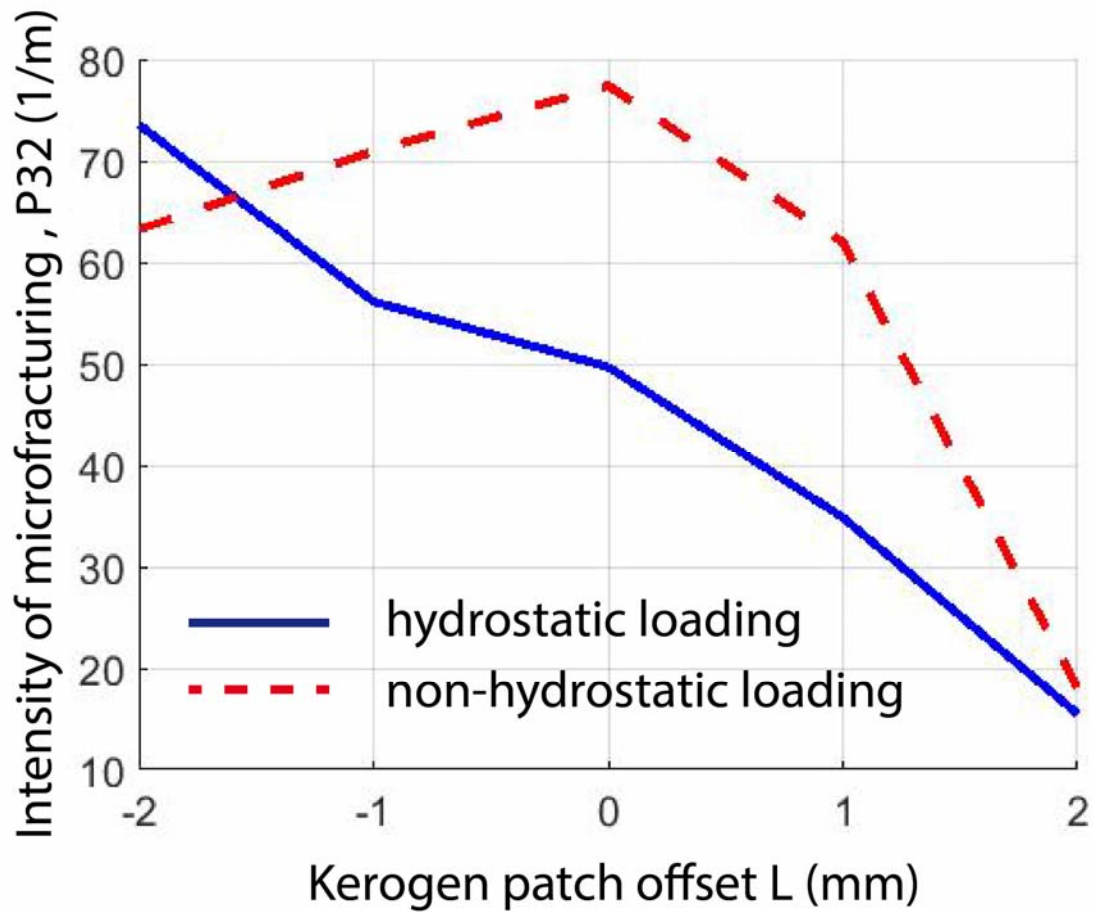
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674 Figure 8: Slice in the middle of the sample showing microfractures (red discs) and fluid
 675 migration (dark cells) for (left) hydrostatic loading with $\sigma_v = 80$ MPa and (right) a differential
 676 stress of 20 MPa with $\sigma_v = 100$ MPa for two kerogen patches with relative vertical offsets $L =$
 677 0 (top) and $L = -2r$ (bottom), where L represents the vertical offset between the two fractures.

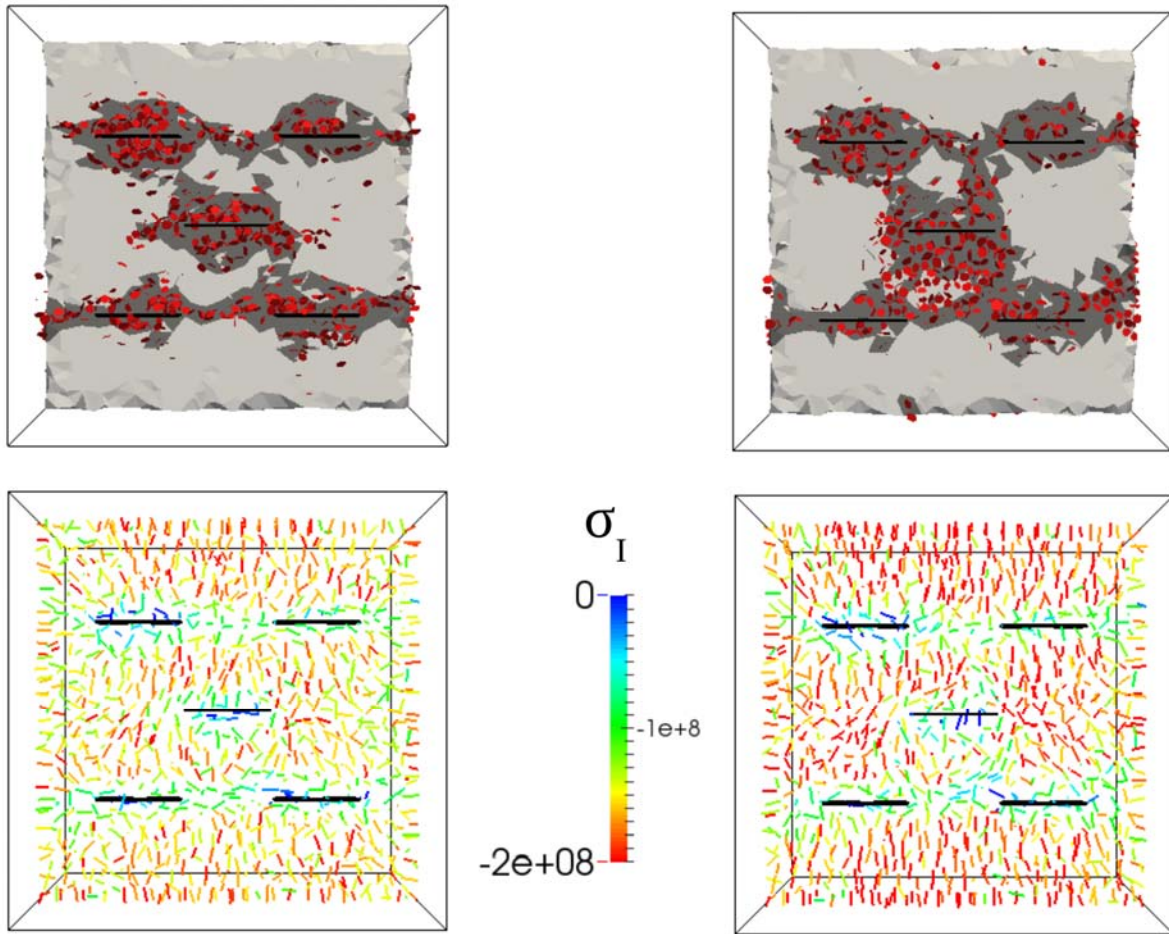
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680 Figure 9: Intensity of microfracturing (parameter P32, see Eq. 1) versus kerogen patch offset
 681 for hydrostatic loading $\sigma_v = 80$ MPa (blue line) and differential-stress loading, $\sigma_v = 100$ MPa
 682 (red dashed line).

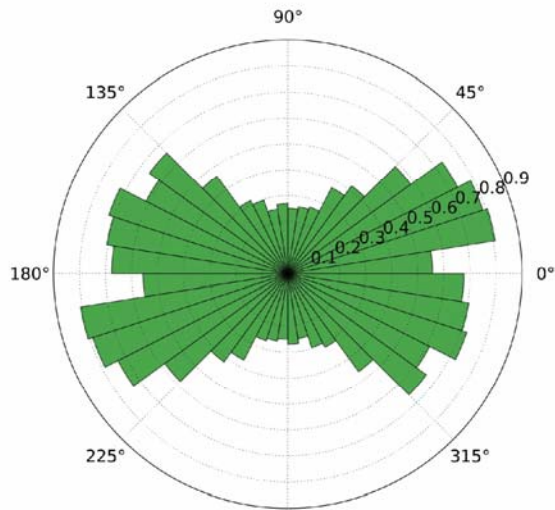
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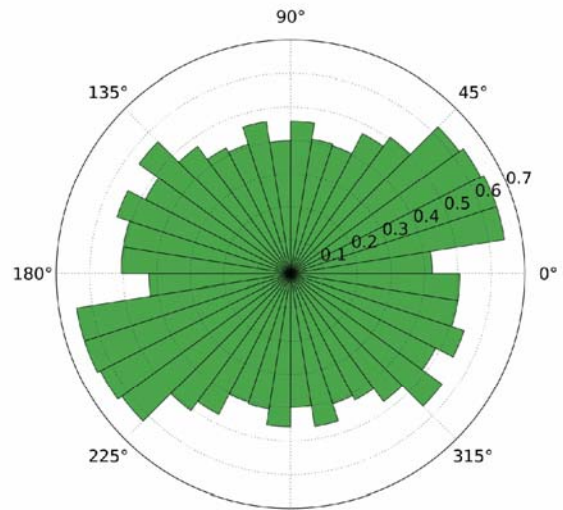
684

685 Figure 10: (top) Slice in the middle of the sample showing microfractures (red discs) and fluid
 686 migration (dark cells) around thirteen horizontal kerogen patches for (left) the hydrostatic case
 687 with $\sigma_v = 80$ MPa and (right) a differential stress of 20 MPa with $\sigma_v = 100$ MPa. (bottom) The
 688 direction and intensity of local maximum principal stress σ_1 (Pa) are represented as thin lines
 689 colored as a function of their intensity for each case.

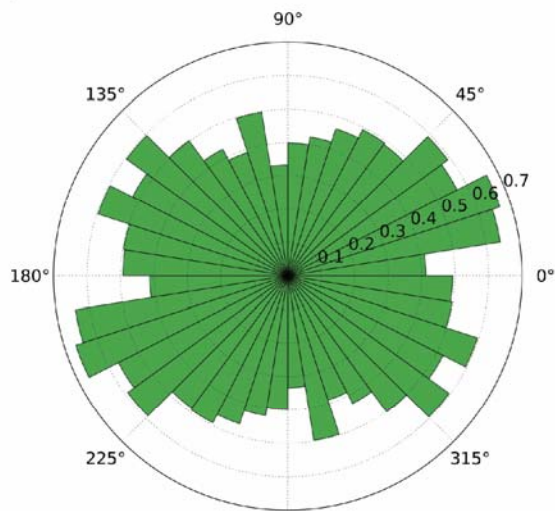
690



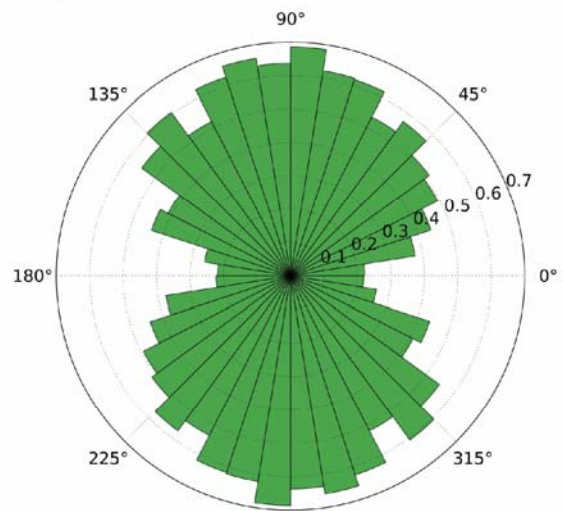
a) $\sigma_v = 80$ MPa (hydrostatic)



b) $\sigma_v = 90$ MPa



c) $\sigma_v = 100$ MPa

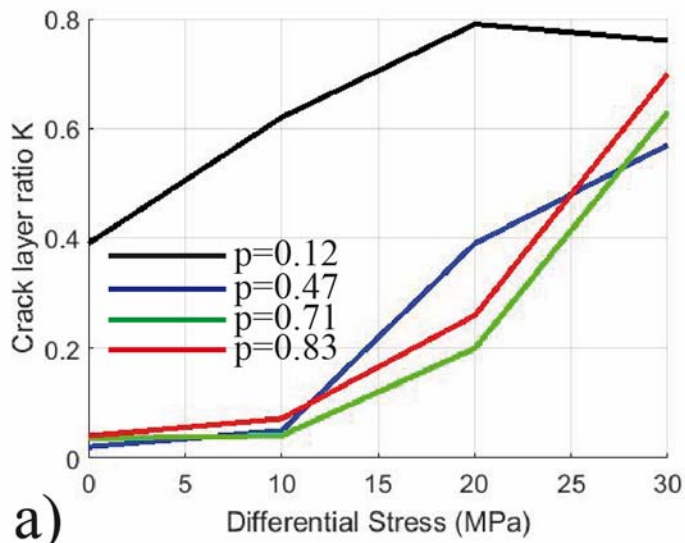


d) $\sigma_v = 110$ MPa

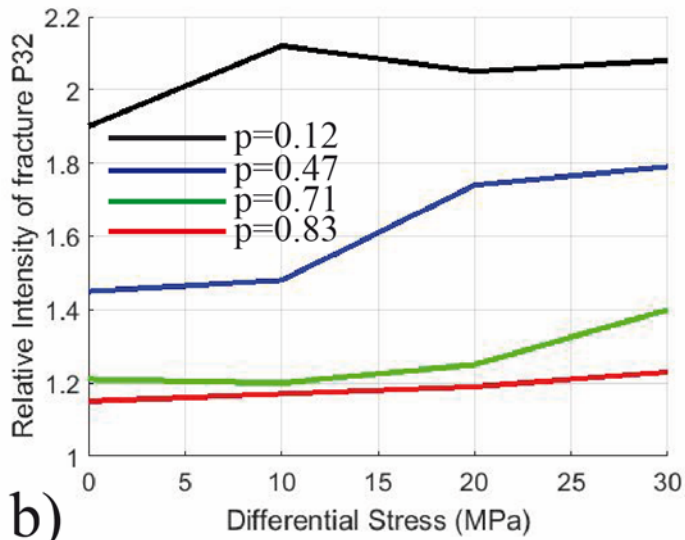
691

692 Figure 11: Normal vector angle of microfractures obtained for simulations with thirteen
 693 kerogen patches. a) $\sigma_v = 80$ MPa (hydrostatic loading); b) $\sigma_v = 90$ MPa; c) $\sigma_v = 100$ MPa; d)
 694 $\sigma_v = 110$ MPa. In all simulations the two horizontal principle stresses are equal to 80 MPa.

695



a)

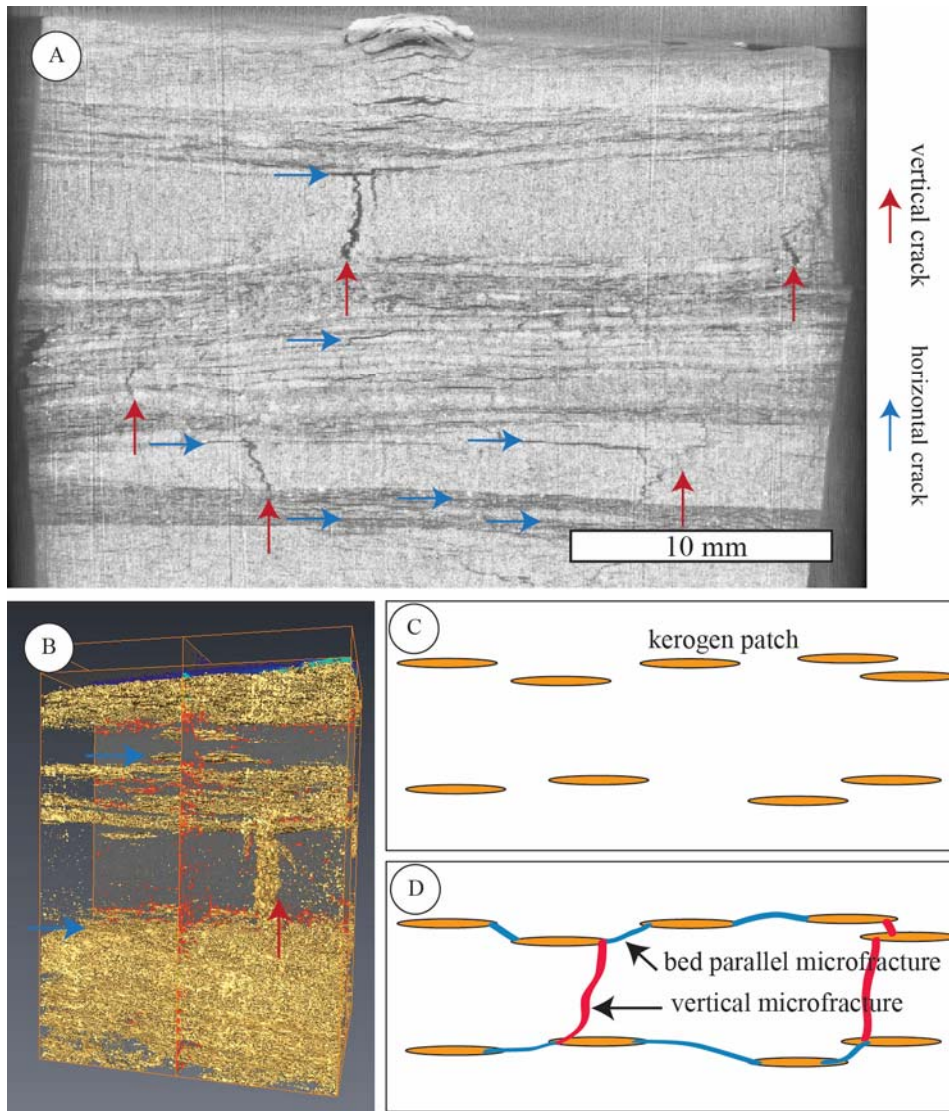


b)

696

697 Figure 12: a) Evolution of the ratio of damage K between kerogen-free and kerogen-rich layers
 698 (see Eq. 2) versus differential stress for different values of the persistence p . b) Evolution of
 699 microfracturing intensity (parameter $P32$, see Eq. 1) versus differential stress for several values
 700 of the persistence p .

701



702

703 Figure 13: a-b) Microtomography views of a shale sample after maturation at 390°C and
 704 differential stress for 24 hours in laboratory conditions. Bed parallel (blue arrows) and bed
 705 perpendicular microfractures (red arrows) for a 3D percolating network. c-d) Conceptual
 706 diagram of the development of a 3D microfracture network and damage creation by the
 707 maturation of organic matter in shales.