

1 Sub-core scale fluid flow behavior in a sandstone with cataclastic deformation bands

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19 Key Points:

- 20 • Cataclastic deformation bands strongly influence the fluid velocity field in a single phase
21 core flooding experiment.
- 22 • Cataclastic deformation bands produce capillary barriers that severely limit cross flow
23 between host rock compartments.
- 24 • The impact of deformation bands, laminae, and experimental boundary conditions are
25 analyzed using numerical simulations.

26 **Abstract**

27 Accurate determination of petrophysical and multiphase flow properties in sandstones is necessary
28 for reservoir characterization, for instance for carbon dioxide and hydrogen storage in geological
29 formations or for enhanced oil recovery. Several studies have examined the effect of
30 heterogeneities, such as fractures, bedding planes and laminae, on core-scale fluid flow. However,
31 the influence of deformation bands that commonly occur in high porosity sandstones, is poorly
32 understood. In this study, we consider a core sample of Navajo sandstone characterized by
33 diagonally oriented deformation bands and two laminae perpendicular to the core axis, as
34 determined from micro X-ray computed tomography (micro-CT). Positron emission tomography
35 (PET) is used to derive the single phase hydrodynamic properties of the core. A CO₂ drainage
36 experiment is conducted in the water-saturated core and imaged with a medical X-ray CT scanner.
37 Medical CT enables CO₂ saturation quantification with increasing CO₂ injection rate.
38 Experimental results and the accompanying numerical simulations indicate that both the laminae
39 and the deformation bands act as capillary barriers, with the laminae forming weaker capillary
40 barriers than the deformation bands. The deformation bands have lower permeability and porosity
41 due to grain crushing, and a very high capillary entry pressure that inhibits CO₂ migration across
42 the bands. At the reservoir scale, deformation bands form conjugate sets and are often present in
43 thick anastomosing clusters that define lozenge-shaped compartments. These findings have
44 important consequences for subsurface fluid flow. For example, the presence of deformation bands
45 may reduce the storage capacity and injectivity in carbon storage reservoirs.

46 **Keywords:** deformation bands, multiphase fluid flow, capillary heterogeneity, X-ray computed
47 tomography, positron emission tomography

48 **Index terms:** Rocks: physical properties, Groundwater transport.

49 **1 Introduction**

50 Sandstones are one of the most high quality and high storage volume candidate geological
51 formations for gas storage due to their global distribution, and high porosity and permeability
52 (Benson & Cook, 2005; Bjørlykke & Jahren, 2010). Key to realizing their potential will be an
53 accurate assessment of their reservoir-scale petrophysical properties and multiphase flow
54 characteristics. These properties govern the behavior of multiphase fluids within the rock and
55 hence will determine the efficiency of injection projects such as carbon dioxide storage, hydrogen
56 storage, and enhanced oil recovery schemes.

57 Together with field observations, laboratory core flooding experiments are a valuable tool for
58 determining petrophysical properties and multiphase flow characteristics under reservoir
59 conditions. Integrating experiments with advanced imaging techniques, such as X-ray computed
60 tomography (CT) and positron emission tomography (PET), enables measurement of single and
61 multiphase flow properties from the pore-scale to the centimeter-scale. In X-ray CT, an X-ray
62 beam is generated, and attenuation values are determined based on the electron density of materials
63 within the sample (Kruth, et al., 2011). This allows the spatial distribution of fluids with differing
64 densities to be determined (Akin & Kovscek, 2003). Both medical CT and micro-CT are
65 commonly used in Earth science. Medical CT is able scan centimeter-scale samples in minutes
66 with millimeter resolution while micro-CT provides micrometer-scale images with scans that take
67 several hours. PET imaging, by contrast, relies on the detection of photons from positron-emitting

68 radiotracers that are injected into the rock. Detection of the photons enables time-resolved
69 quantification of radiotracer migration through the sample. Thus with PET imaging it is possible
70 to quantify fluid transport behavior, while CT provides high-resolution information about rock
71 structure and fluid saturation distribution (Pini, et al., 2012; Zahasky, et al., 2019).

72 Imaging and analysis of core flooding experiments enables quantification of rock and fluid
73 properties, such as porosity and absolute permeability (Krause, et al., 2013; Ochi & Vernoux,
74 1998; Perrin, et al., 2009; Zahasky & Benson, 2018), fluid saturation, capillary pressure and
75 relative permeability (Akbarabadi & Piri, 2013; Krevor, et al., 2012; Pini, et al., 2012; Ruprecht,
76 et al., 2014; Vinegar & Wellington, 1987). Many of these studies indicated that sandstones are
77 characterized by subtle small-scale heterogeneities that actively affect fluid flow. Variations in
78 porosity and permeability affect the fluid velocity field, with high velocities being associated with
79 regions of high porosity and permeability (Bloomfield, et al., 2001; Grathwohl & Kleineidam,
80 1995; Vasco, et al., 2018; Zahasky & Benson, 2018) and for multiphase fluid flow, variations in
81 capillary pressure and relative permeability affect plume migration and residual saturation at both
82 the pore and the field scale (Hingerl, et al., 2016; Krevor, et al., 2012; Krevor, et al., 2015; Li &
83 Benson, 2015; Perrin & Benson, 2010; Pini & Benson, 2017; Saadatpoor, et al., 2010). In
84 particular, Krevor et al. (2011) reported that regions presenting high capillary entry pressures (i.e.
85 small pore throats) act as capillary barriers for the non-wetting fluid, leading to an increase in
86 saturation of the latter in the preceding pores.

87 Until now, sub-core scale flow and transport behavior in heterogeneous porous media has focused
88 on sandstones characterized by the presence of bedding planes, laminae and/or fractures (Corey &
89 Rathjens, 1956; Hingerl, et al., 2016; Kim, et al., 2018; Krevor, et al., 2011; Li, et al., 2019;
90 Manzocchi, et al., 2002; Medina, et al., 2011; Pasala, et al., 2013; Shipton, et al., 2002;
91 Tueckmantel, et al., 2012). Relatively little attention has been given to experimentally
92 understanding the impact of deformation bands on fluid flow. Deformation bands are low porosity
93 bands that form in response to shear and they are extremely common in sandstones with a porosity
94 greater than 0.15 (Aydin, 1978; Fossen, et al., 2007; Schultz & Siddharthan, 2005). Several types
95 of deformation bands can be defined based on their kinematic mechanisms. The most common are
96 compactional shear or cataclastic bands (Aydin, et al., 2006). These form by a combination of
97 shear and compaction mechanisms and are always characterized by cataclasis. Cataclastic bands
98 are millimeters thick tabular structures (Aydin, 1978; Aydin & Johnson, 1978), along which grain
99 rolling and grain fracturing lead to a reduced porosity and permeability. Multiple studies have
100 reported that deformation bands are several orders of magnitude less permeable than the host rocks
101 in which they form (Antonellini & Aydin, 1994; Aydin & Johnson, 1978; Ballas, et al., 2015;
102 Fossen, et al., 2007; Taylor & Pollard, 2000). A single band can accommodate only a few
103 millimeters of displacement; upon further deformation, rather than continuously slipping, a pre-
104 existing band experiences strain hardening (Aydin & Johnson, 1978; Shipton & Cowie, 2003). As
105 a result, new bands form to accommodate additional strain. This is why conjugate sets or
106 anastomosing clusters of deformation bands are common.

107 Cataclastic bands usually form at burial depths greater than 1 km, but there is evidence of their
108 presence at shallower burial depths in unconsolidated sandstones (Cashman & Cashman, 2000;
109 Rawling & Goodwin, 2003). They are often found in fault damage zones, i.e. in the volume of
110 rock that accommodates deformation during initiation and propagation of slip along fault
111 (McGrath & Davison, 1995; Rotevatn & Fossen, 2011; Shipton & Cowie, 2001; Shipton & Cowie,

112 2003). Since deformation bands are well below the resolution of seismic data, their extent within
113 the damage zone is not easy to predict (sub-seismic faults are generally faults with an offset of <
114 10 m that cannot be detected using seismic reflection data, although strike slip faults of much
115 larger offsets are also not resolvable). Moreover, it has been found that no relationship exists
116 between fault displacement and frequency of deformation bands (Schueller, et al., 2013): the same
117 frequency of deformation bands may be associated with seismically resolvable faults and sub-
118 seismic faults.

119 It is highly likely that deformation bands will be present in most high porosity sandstone reservoirs,
120 hence understanding how they influence fluid flow, and determining their petrophysical properties,
121 is key to accurate reservoir characterization. Several studies have highlighted how deformation
122 bands can negatively affect fluid flow, leading to pressure compartmentalization, a higher degree
123 of tortuosity, fluid bypass and a lower than expected reservoir permeability (Ogilvie, et al., 2001;
124 Qu & Tveranger, 2016; Rotevatn & Fossen, 2011; Rotevatn, et al., 2017; Schultz & Siddharthan,
125 2005; Shipton, et al., 2002; Shipton, et al., 2005; Wilkins, et al., 2019). However, most of these
126 studies have relied on results from reservoir simulations and analysis of field data. Here, we present
127 the first *in situ* visualization and quantification of sub-core scale single phase and multiphase fluid
128 flow experiments in a sandstone rock core that contains deformation bands and fine-grained
129 laminae. Laminae are mm-thick sedimentary layers forming due to episodic changes in
130 depositional energy (Campbell, 1967). Single phase flow experiments were conducted using PET
131 imaging. Multiphase flow experiments were performed by injecting CO₂ into a water saturated
132 rock sample and acquiring several consecutive medical X-ray CT scans. Our results demonstrate
133 that deformation bands significantly influence single phase flow and that in a multiphase flow
134 setting, they have a profound effect on fluid phase distribution within the rock.

135 **2 Methodology**

136 The 5 cm diameter, 10 cm long rock core used in this study was retrieved from a borehole depth
137 of 57 m in the Navajo sandstone formation. The borehole was drilled into the hanging wall of the
138 Big Hole normal fault, in the north of the San Rafael Swell, Utah (Shipton, et al., 2002). The core
139 was sampled from the 17 m thick damage zone that surrounds the Big Hole Fault at this location.
140 The host rock is characterized as a fine-grained sandstone with cataclastic deformation bands
141 (Figure 1a).

142 *2.1 Micro-CT*

143 To characterize the geometry of the deformation bands, the core was scanned at the University of
144 Strathclyde with an X-ray micro-CT scanner (Nikon XT H 225 LC) that produced three-
145 dimensional (3D) tomographic images with a voxel size of 0.029x0.029x0.029 mm. The above
146 mentioned facility was, however, not available for imaging during the core flooding experiments.
147 Core flooding experiments were conducted at Stanford University using medical CT and PET
148 imaging. The high-resolution micro-CT images provide more detailed information on the
149 deformation band geometries that could not be inferred by the lower resolution of medical CT and
150 PET scanner.

151 *2.2 Porosity characterization*

152 The 3D porosity distribution within the core was determined using a medical X-ray CT scanner
153 (General Electric Hi-Speed CT/i) at Stanford University. Image acquisition was performed at 120

154 kV and 200 mA, obtaining a voxel dimension of 0.3125x0.3125x0.625 mm. Images of the core
 155 were taken when fully dry (CT_{dry}) and when fully water saturated (CT_{water}). The porosity, Φ ,
 156 was then calculated using the following relationship (Withjack, 1988; Akin & Kovscek, 2003):

$$157 \quad \Phi = \frac{CT_{water} - CT_{dry}}{I_{water} - I_{air}} \quad (1)$$

158 where I_{water} and I_{air} are the water and air X-ray attenuation values respectively, which differ
 159 by 1000 Hounsfield units (Wellington & Vinegar, 1987). To reduce noise in CT images at least
 160 three series for each condition were acquired and averaged (Pini, et al., 2012). The images of the
 161 entire core were discretized into 38x38x76 cells, each with a dimension of 0.125 cm.

162 2.3 Single phase permeability characterization

163 Bulk intrinsic permeability was determined using the core-flooding set-up described in the section
 164 2.4 and under the same conditions of temperature, pressure and confining pressure as for the
 165 multiphase flow experiment. Injecting water at several flow rates into the water saturated core
 166 sample and measuring corresponding differential pressure across the core, allowed permeability
 167 calculation with Darcy's Law.

168 To investigate the 3D distribution of permeability within the core, a tracer experiment was
 169 conducted within the micro-PET scanner (Siemens Inveon D-PET) using the experimental setup
 170 described in Zahasky & Benson (2018). Before fluid injection, the core was wrapped in two heat-
 171 shrinkable Teflon layers and a rubber sleeve to avoid any leakage of the confining fluids into the
 172 core. The core was then placed in an aluminum core holder with inlet and outlet caps etched with
 173 a pattern of connected grooves for an even distribution of injected fluids. Finally, the core holder
 174 was placed in the micro-PET scanner and connected to the core flooding equipment.

175 To ensure full core water saturation, the core was first dried. CO₂ was then injected to displace the
 176 air, followed immediately by water that was injected for displacing and dissolving the CO₂. Once
 177 the core was fully saturated, a solution of Fludeoxyglucose (¹⁸F-FDG) diluted in tap water was
 178 injected at 4 mL/min. The approximate radioactive concentration was 0.52 mCi/mL. Throughout
 179 the experiment a PET scan continuously acquired photon detection data. The experiment was
 180 carried out at a constant temperature of 20 °C, with a confining pressure of 2.4 MPa. The back
 181 pressure was maintained just above atmospheric pressure.

182 To calculate the 3D concentration field of the radiotracer within the core, the PET scan data was
 183 reconstructed with a time-step length of 40 seconds. The image-based core was discretized into a
 184 grid of 22x22x42 cells giving a voxel size for each concentration measurement of 0.23x0.23x0.23
 185 cm. Analyzing concentration measurements as a function of time from the PET scans, enables
 186 estimates of the mean arrival time and fluid velocity at any location within the core. The radiotracer
 187 concentration in each voxel over time was fitted with a first order Gaussian function to remove
 188 background noise (Vasco, et al., 2018). The total mass of radiotracer was calculated for each voxel
 189 using the temporal zero moment equation

$$190 \quad M0 = \int_0^t c \, dt \quad (2)$$

191 where c is the radiotracer concentration in each voxel. The mean arrival time is identified as the
 192 center of mass of the Gaussian function and calculated with the temporal first moment equation
 193 (Naff, 1990).

$$194 \quad M1 = \int_0^t ct \, dt \quad (3)$$

195 The normalized first moment then defines the mean arrival time of the plume center.

$$196 \quad nM1 = \frac{M1}{M0} \quad (4)$$

197 Knowing the distance between two adjacent units, i.e. the distance between voxels, a map of the
 198 velocity field can be derived. The velocity is normalized, enforcing a mass balance, by setting the
 199 total flow rate of each cross-sectional slice within the core equal to the inflow rate that we imposed
 200 in the experiment (4 mL/min). This analysis assumes flow is parallel to the axis of the core, a good
 201 approximation as the cylindrical faces of the core were no-flow boundaries.

202 *2.4 Multiphase core flooding experiments*

203 To determine the multiphase flow properties of the rock core, CO₂/water drainage capillary
 204 pressure experiments (Pini, et al., 2012) at steady-state conditions were conducted at 25 °C and 9
 205 MPa, with a confining pressure of 11 MPa. Drainage is the process of displacing the wetting phase
 206 (water) with non-wetting phase (CO₂). Near ambient temperature was used here because previous
 207 studies have shown that temperature has no influence on the saturation end point when CO₂ is
 208 injected in a water saturated sample (Niu, et al., 2015). The core flooding setup is similar to the
 209 one used in previous experiments (Krevor, et al., 2012; Ni, et al., 2019; Perrin & Benson, 2010)
 210 and details can be found in supporting information (Text S1, Figure S1). The core was not fired
 211 before the experiment, due to the low clay content (Shipton, et al., 2002) and because previous
 212 studies have shown that firing in CO₂/water/sandstone (with low clay content) system does not
 213 change experimental results and wetting properties (Garing & Benson, 2019). The core was first
 214 dried in the oven for several days and then wrapped using the same layering protocol as for the
 215 single phase experiment (section 2.3). Considering that CO₂ can permeate through Teflon, an
 216 additional layer of aluminum foil has been placed between the Teflon layers to avoid any radial
 217 diffusion of CO₂ out of the rock core. The core was then placed in an aluminum core holder and
 218 connected to a core flooding setup suitable for conducting high pressure and temperature-
 219 controlled experiments.

220 Before CO₂ injection, the rock core was fully saturated with water that had been pre-equilibrated
 221 with CO₂ at the experimental conditions. For the drainage experiment, 100% CO₂ was
 222 continuously injected at progressively higher flow rates, from 0.3 mL/min to 20 mL/min. At these
 223 conditions the capillary number $Ca = \frac{v \mu_{CO_2}}{\gamma}$ ranges from 10⁻⁷ to 10⁻⁸, where v is the fluid velocity
 224 (m/s), $\mu_{CO_2} = 7.06 \times 10^{-5}$ (Pa · s) is the viscosity of the CO₂ at experimental conditions and $\gamma = 35$
 225 (mN/m) is the CO₂/water interfacial tension. This suggests that capillary forces dominate over
 226 viscous forces in this system. A Bond number, $Bo = \frac{\Delta\rho g L^2}{\gamma}$ (density difference $\Delta\rho$ of 201 kg·m⁻³
 227 and a pore length L of 50 micron) on the order of 10⁻⁵ indicates that buoyancy forces are smaller
 228 compared to capillary forces.

229 At each flow rate each flow rate, a minimum of 5 PV (1 PV = 38 mL) of CO₂ were injected to
 230 ensure steady state was reached (Perrin, et al., 2009). Once steady state conditions were reached,
 231 the medical X-ray CT scanner (section 2.2) was used for obtaining scan images of the CO₂
 232 saturated core, water saturated core and partially saturated core with a voxel size of
 233 0.3125x0.3125x0.625 mm. CO₂ saturation (S_{CO_2}) is measured using the following formula (Akin
 234 & Kovsky, 2003):

$$235 \quad S_{CO_2} = \frac{CT_{exp} - CT_{wat sat}}{CT_{CO_2 sat} - CT_{wat sat}} \quad (5)$$

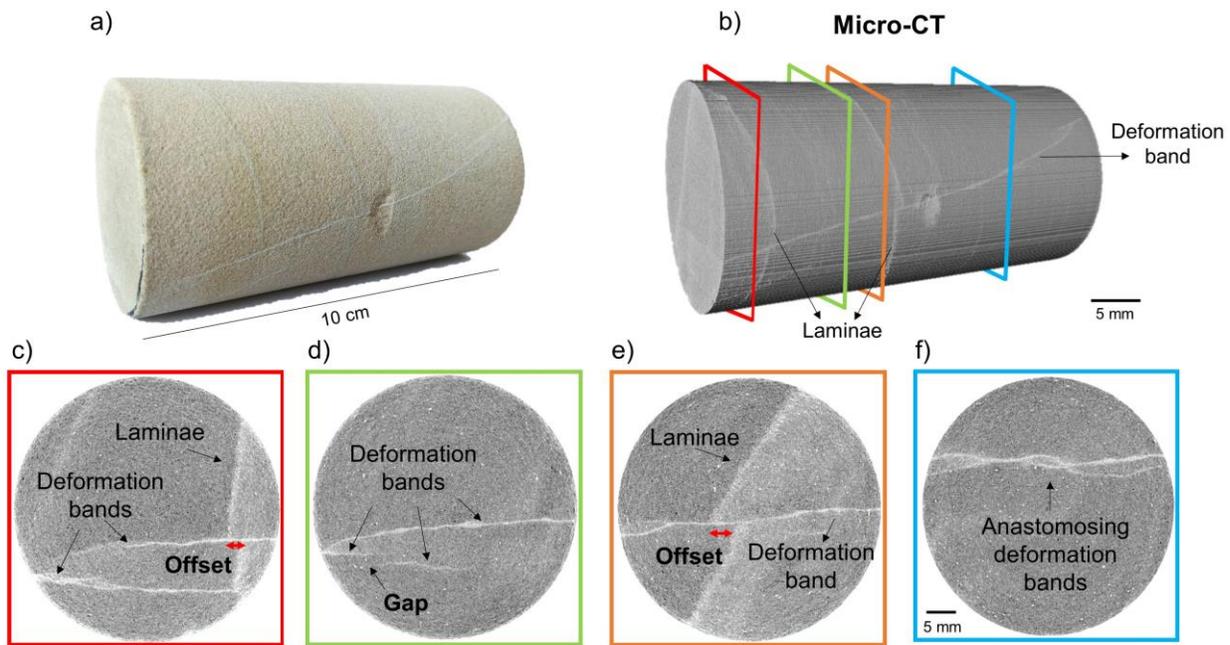
236 where $CT_{wat sat}$ are scan images taken when the core was fully saturated with equilibrated water,
 237 $CT_{CO_2 sat}$ are the scan images of the fully CO₂ saturated core. For each condition, at least three
 238 series of scans were taken; and the average of the three was computed for reducing uncertainties
 239 on saturation results (Pini, et al., 2012). The resulting images were then coarsened for further noise
 240 reduction, obtaining a final voxel resolution of 0.125x0.125x0.125 cm.

241 Capillary pressure at the inlet portion of the core was measured for each flow rate as the difference
 242 between the core inlet and outlet pressure readings. This assumes that during steady state CO₂
 243 injection the pressure recorded at the inlet is the CO₂ pressure and the pressure recorded at the
 244 outlet is the water pressure (Pini, et al., 2012).

245 **3 Results**

246 *3.1 Deformation band geometry*

247 Figures 1a and 1b show a photograph of the core alongside a 3D image of the distribution of
 248 attenuation values from the X-ray micro-CT scanner: higher attenuation values, in white,
 249 correspond to higher density materials. A deformation band is clearly visible in both images
 250 traversing the full sample horizontally from end-to-end, at an angle of approximately 18° to the
 251 long-axis of the core. Two core-perpendicular laminae of finer grained material are also apparent
 252 in the micro-CT scan (Figure 1b). Analysis of sequential cross-sectional slices in the X-ray micro-
 253 CT scan (Figures 1c-1f) show that, rather than a single band, there are two bands. These offset the
 254 first and second laminae by 3 mm and 5 mm respectively in the slice shown in Figures 1c and 1e.
 255 On all the X-ray micro-CT slices, the two main deformation bands are separated by host rock and
 256 therefore they do not isolate any portion of the core (Figure 1d). Toward the end of the core (Figure
 257 1f), only one deformation band is present, which takes the form of a small anastomosing cluster.

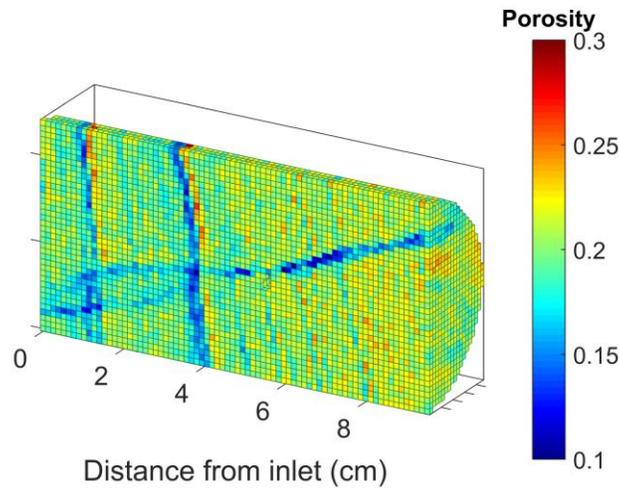


258

259 **Figure 1.** a) Sandstone core sample with cataclastic diagonal deformation band. b) 3D micro-CT
 260 scan of the sandstone core: the sample is characterized by a cataclastic deformation band and
 261 laminae. Raw data are available in the data repository cited in the Acknowledgments. c) 2D Slice
 262 image showing that the two deformation bands offset the first lamina by 3 mm. Deformation bands
 263 do not connect to each other on the left side of the image. d) A third deformation band appears in
 264 this slice. The bands are not joined and hence they do not form any isolated compartments. e)
 265 Second lamina cut by a single deformation band. Offset of about 5 mm. f) Small anastomosing
 266 network of deformation bands at the end of the core.

267 3.2 Porosity distribution

268 The distribution of porosity within the core, based on the dry and water saturated medical X-ray
 269 CT scans (section 2.2), is shown in Figure 2. The deformation bands and laminae are clearly visible
 270 as low porosity features. Bulk porosity of the core was calculated as 0.196. Deformation band
 271 porosity ranges from 0.07 to 0.15, while porosity of laminae varies from 0.13-0.15.

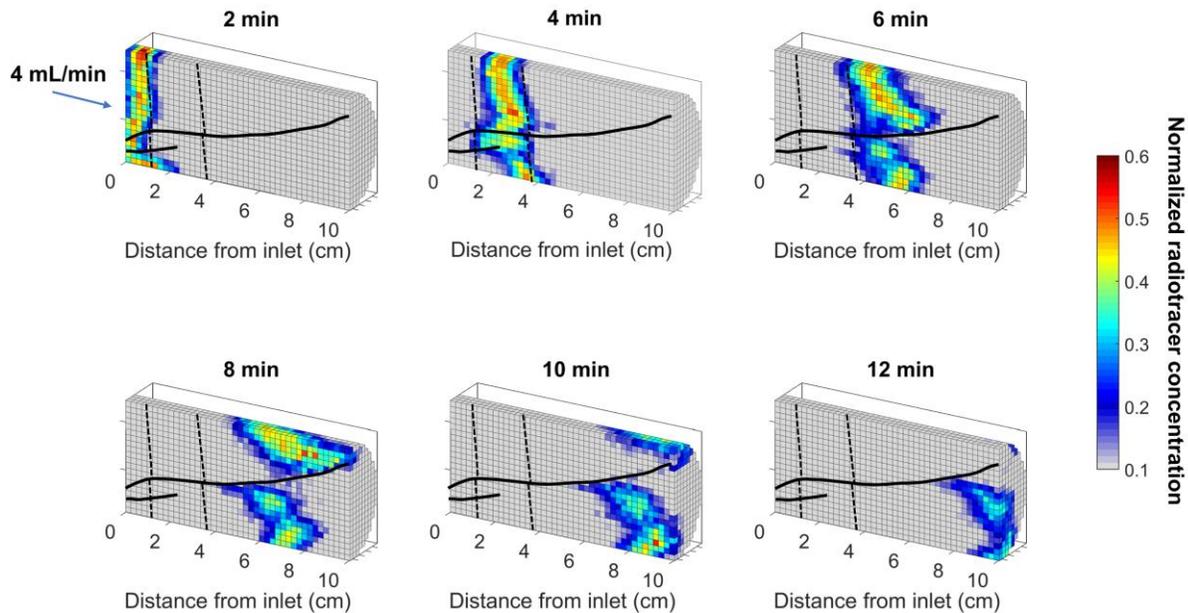


272

273 **Figure 2.** Porosity map calculated by using water saturated and dry scan images with the medical
 274 X-Ray CT scanner. Voxel resolution 0.125x0.125x0.125 cm. An uncertainty (σ_ϕ) of 0.0082 in
 275 voxel porosity due to random error of CT number was calculated using methods explained in Pini
 276 et al. (2012).

277 *3.3 Intrinsic permeability*

278 Based on measurement of the inlet and outlet pressures at a constant flow rate, a bulk sample
 279 permeability of 53 mD was estimated using Darcy's Law. The heterogeneous distribution of
 280 permeability within the core was investigated using the PET scanner. Figure 3 shows the
 281 concentrations of the single phase radiotracer injection experiment during six different timeframes
 282 of the PET scan taken at consecutive 2-minute intervals. Stylized deformation bands and laminae
 283 (derived from the micro-CT images) have been superimposed on the PET images to illustrate their
 284 effect on the tracer plume migration. Results show that the tracer plume above and below the bands
 285 is beginning to diverge 4 min after the start of injection. This effect is more pronounced with
 286 increasing distance from the inlet. There is a very low radiotracer concentration in the volume of
 287 rock that immediately surrounds the bands.



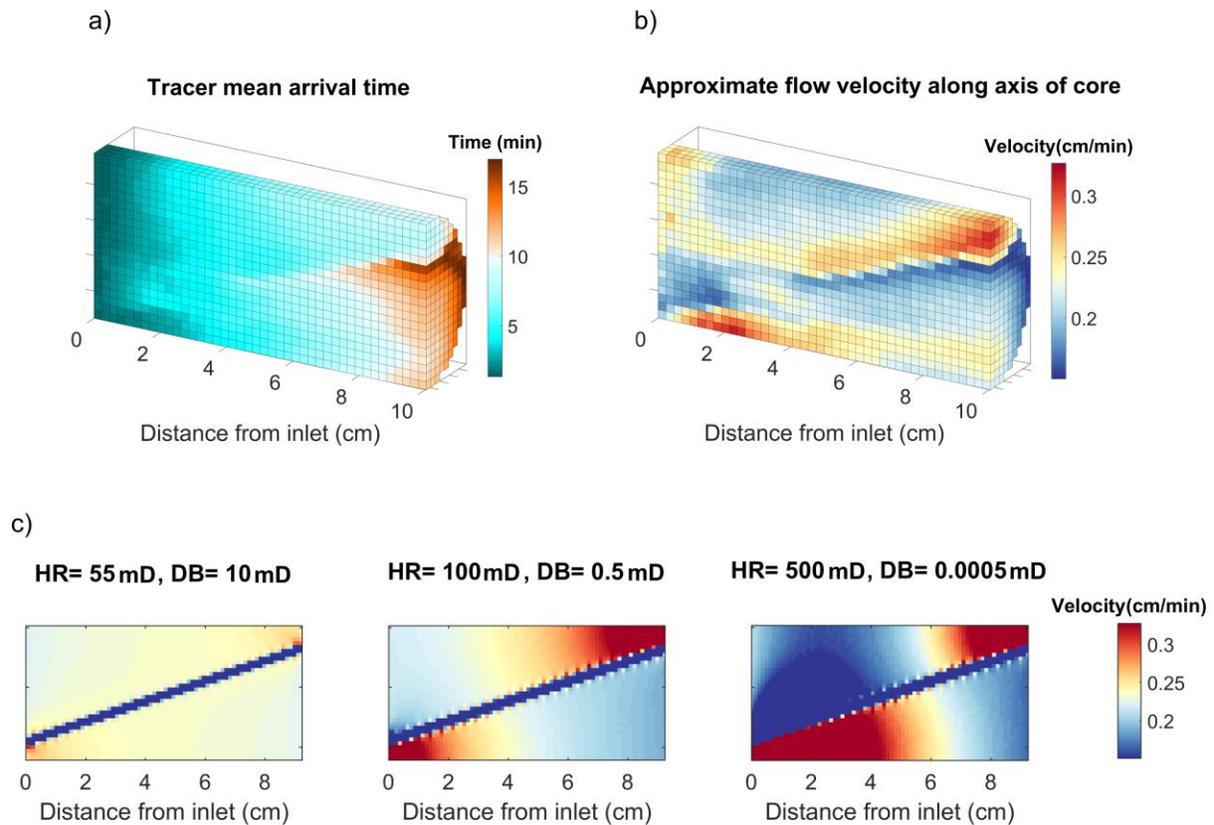
288

289 **Figure 3.** Axial plane snapshots of radiotracer concentration measured at 2-minute time intervals
 290 after injection at 4 mL/min into a sandstone core with deformation bands. The approximate
 291 deformation bands (continuous black lines) and laminae (dashed black lines) locations are
 292 superimposed on the PET images. Voxel size is 0.23x0.23x0.23 cm.

293 The 3D map of mean arrival time calculated from the PET images (Figure 4a) shows a significantly
 294 delayed arrival time for the portion of the host rock that is below the deformation bands compared
 295 to above. In the corresponding 3D map of fluid velocity (Figure 4b) there is a clear distinction
 296 between velocity in the rock above and below the deformation bands. These differences are related
 297 to the geometry of the deformation band within the sample. The deformation band, along which
 298 the estimated velocity is almost zero, subdivides the host rock into two regions. In the upper region,
 299 the cross-sectional area decreases towards the outlet and hence, according to the principle of
 300 continuity, if the flow rate is held constant, the velocity increases. Vice-versa for the region below
 301 the bands, the cross-sectional area increases towards the outlet and, hence, the fluid velocity
 302 decreases. In both the estimated mean arrival time (Figure 4a) and the velocity (Figure 4b) maps
 303 there is no discernable effect of the two sub-vertical laminae on flow.

304 To estimate the mean intrinsic permeability for both the host rock and the deformation bands, the
 305 PET experiment was modelled numerically using the Stanford University General Purpose
 306 Research Simulator software (GPRS) (Cao, 2002; Jiang, 2008; Li, 2011; Boon, et al., 2018; Cao
 307 & Aziz, 2002; Krause, 2012; Krause, et al., 2013; Li, et al., 2012; Li & Benson, 2015). Details of
 308 model set-up are included in supporting information (Table S1, Figure S2). Multiple combinations
 309 of the host rock permeability and deformation band permeability were tested. Each combination
 310 had an equivalent bulk core permeability equal to the experimentally measured value of 53 mD.
 311 Flow within the core was modelled in 2D, using a grid of 35X78 cells with a grid cell resolution
 312 of 0.125 cm, a homogeneous host rock and a single, straight, diagonal deformation band (Figure

313 4c). The velocity of the fluid for each cell in the simulations was calculated using Darcy's law,
 314 assuming an axial flow direction. The simulation results for three combinations of host rock and
 315 deformation band permeability are shown in Figure 4c. Specifically, the combinations evaluated
 316 were 55 mD and 10 mD, 100 mD and 0.5 mD, 500 mD and 0.0005 mD for the host rock and
 317 deformation band respectively. A qualitative comparison of the velocity fields calculated from
 318 model simulations with the PET-derived velocity field shows that, although all three models have
 319 the same bulk permeability, the local velocity distributions differ. The results for a permeability of
 320 100 mD for the host rock and 0.5 mD for the deformation band most closely resemble the
 321 experimental data (Figure 4b).



322

323 **Figure 4.** a) Mean arrival time of the radiotracer solution in the sandstone core with deformation
 324 bands. Delayed arrival time in compartment below the deformation bands. b) Fluid velocity along
 325 the axis of the core calculated from the experimental data. c) Fluid velocity calculated simulating
 326 water injection in three pseudo 3D models with different permeability in the host rock (HR) and
 327 deformation band (DB). The model with 100 mD in the HR and 0.5 mD in the DB provides the
 328 best match with the velocity field obtained in the experiments.

329 The heterogeneous permeability distribution was estimated using the porosity-permeability
 330 relationship proposed by Torabi et al. (2013):

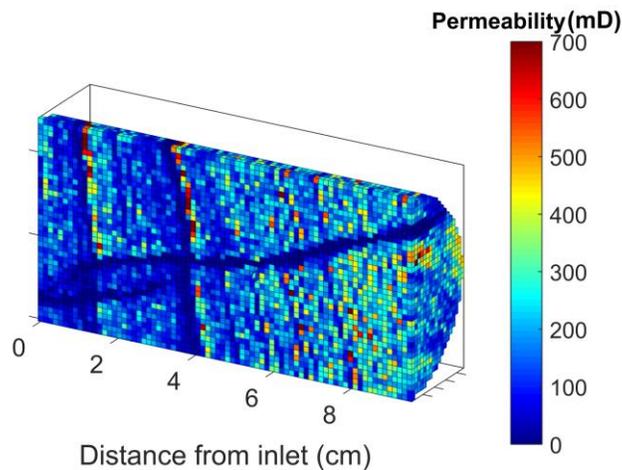
331

$$k_{HR} = 1e - 9 \varphi_{HR}^{AHR} \quad (6)$$

332

$$k_{DB} = 2e - 7\varphi_{DB}^{ADB} \quad (7)$$

333 where k_{HR} , φ_{HR} , k_{DB} , φ_{DB} are permeability (mD) and porosity (in percentage) of the host rock
 334 and deformation bands respectively and A_{HR} and A_{DB} are dimensionless constants. Among several
 335 porosity-permeability relationships, this is preferred considering that it specifically relies on core-
 336 plug laboratory measurements of undeformed and deformed samples (single and clusters of bands).
 337 For our specific study, porosity for each voxel in the core was taken from the data in Figure 2. The
 338 A_{HR} and A_{DB} coefficients found by Torabi et al. (2013) are 9.09 and 6.31, respectively. However,
 339 by using these coefficients the resulting bulk core permeability, calculated performing single phase
 340 simulations, was 280 mD as opposed to the 53 mD experimentally calculated. The constants A_{HR}
 341 and A_{DB} were then fitted by constraining the bulk core permeability to have the measured value of
 342 53 mD and the bulk host rock and deformation band permeabilities to have values of 100 mD and
 343 0.5 mD respectively, as estimated from the analysis shown in Figure 4. This resulted in estimates
 344 for the constants A_{HR} and A_{DB} of 8.6 and 5.4 for the host rock and deformation bands respectively.
 345 The estimated permeability in each cell is shown in Figure 5.



346

347 **Figure 5.** Permeability distribution in millidarcy (mD) calculated using an adapted version of the
 348 porosity-permeability relationship found in Torabi et al. (2013).

349 3.4 Multiphase flow properties

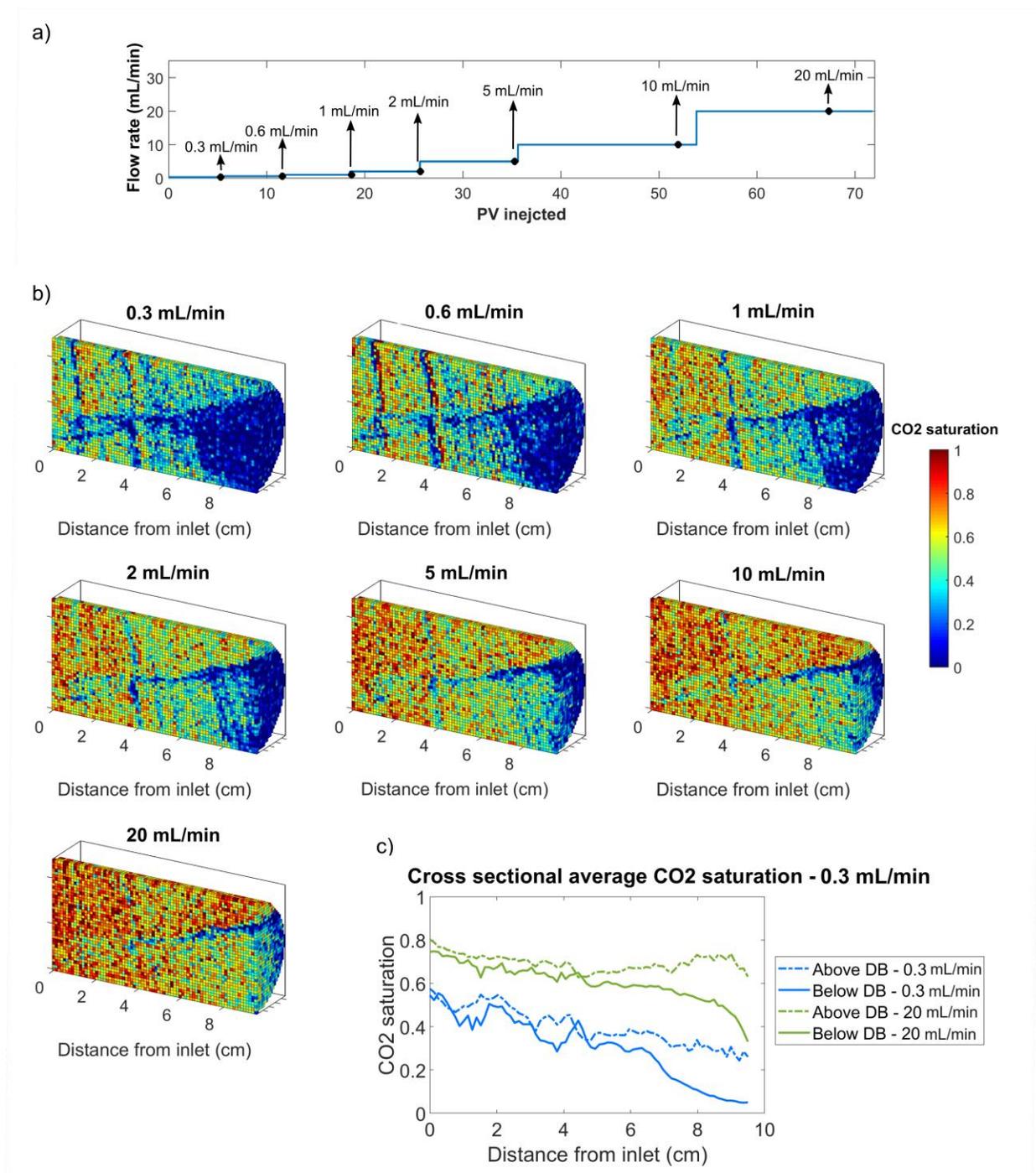
350 Results of the core flooding CO_2 injection experiments are shown in Figure 6. The injection flow
 351 rate was steadily increased in a step-wise fashion over time (Figure 6a). At each step, the flow rate
 352 was maintained for a sufficient duration to achieve a steady-state CO_2 saturation distribution (as
 353 determined from consecutive medical CT scans). Figure 6b shows that as the flow-rate increases,
 354 CO_2 saturation increases in the host rock compartments above and below the deformation bands,
 355 but that there remains a lower CO_2 saturation in the compartment below the bands. At low flow
 356 rates (0.3 mL/min – 0.6 mL/min – 1 mL/min – 2 mL/min) CO_2 is not able to saturate the outlet of
 357 the core below the deformation bands, creating a shadow zone of reduced CO_2 saturation.

358 Due to their low porosity and permeability and high capillary entry pressure, the deformation bands
 359 exhibit low CO_2 saturation, even at high flow rates. Flow across the bands can only occur if the

360 capillary entry pressure of the bands has been exceeded. Hence, the bands act as capillary barriers
361 and inhibit most flow between the two compartments even at high flow rates.

362 In contrast to the single phase PET tracer experiment (Figure 3), the laminae have a visible effect
363 on CO₂ distribution, with CO₂ saturation being lower in the laminae than the surrounding host
364 rock. The laminae also act as capillary barriers, although to a lesser extent than the deformation
365 bands. Saturation in the laminae remains lower than in the surrounding rock even when the
366 saturation front has passed through the bands. Only once the flow rate reaches 5 mL/min do the
367 laminae fully saturate and at that point they are no longer clearly visible in the X-ray CT images.

368 The slice-averaged CO₂ saturation for the individual host rock compartments (Figure 6c) indicates
369 that the CO₂ saturation is lower in the compartment below the bands compared to above the bands.
370 This discrepancy becomes less pronounced at the high flow rates. Despite this, even at 20 mL/min
371 of CO₂ injection, the portion of the core near the inlet shows a lower CO₂ saturation in the
372 compartment below the bands.



373

374 **Figure 6.** a) Injection strategy for the core flooding drainage experiments. CO₂ was injected in the
 375 water saturated sample at progressively higher flow rates of 0.3, 0.6, 1, 2, 5, 10, 20 mL/min. Circle
 376 marks corresponds to the scan images taken at steady state conditions for each flow rate. b) CO₂
 377 saturation measured for different flow rates at steady state conditions. Voxel resolution
 378 0.125x0.125x0.125 cm. Grid size is 38x38x76 cells. c) Slice average CO₂ saturation for the
 379 compartment below and above the deformation bands (DB) for both flow rates, 0.3 mL/min and
 380 20 mL/min. The difference in saturation between the two compartments is higher towards the

381 outlet and less pronounced for the highest flow rate. An uncertainty of 0.18 in voxel saturation
382 measurement (σ_s) due to random error of CT number was calculated using methods explained in
383 Pini et al. (2012).

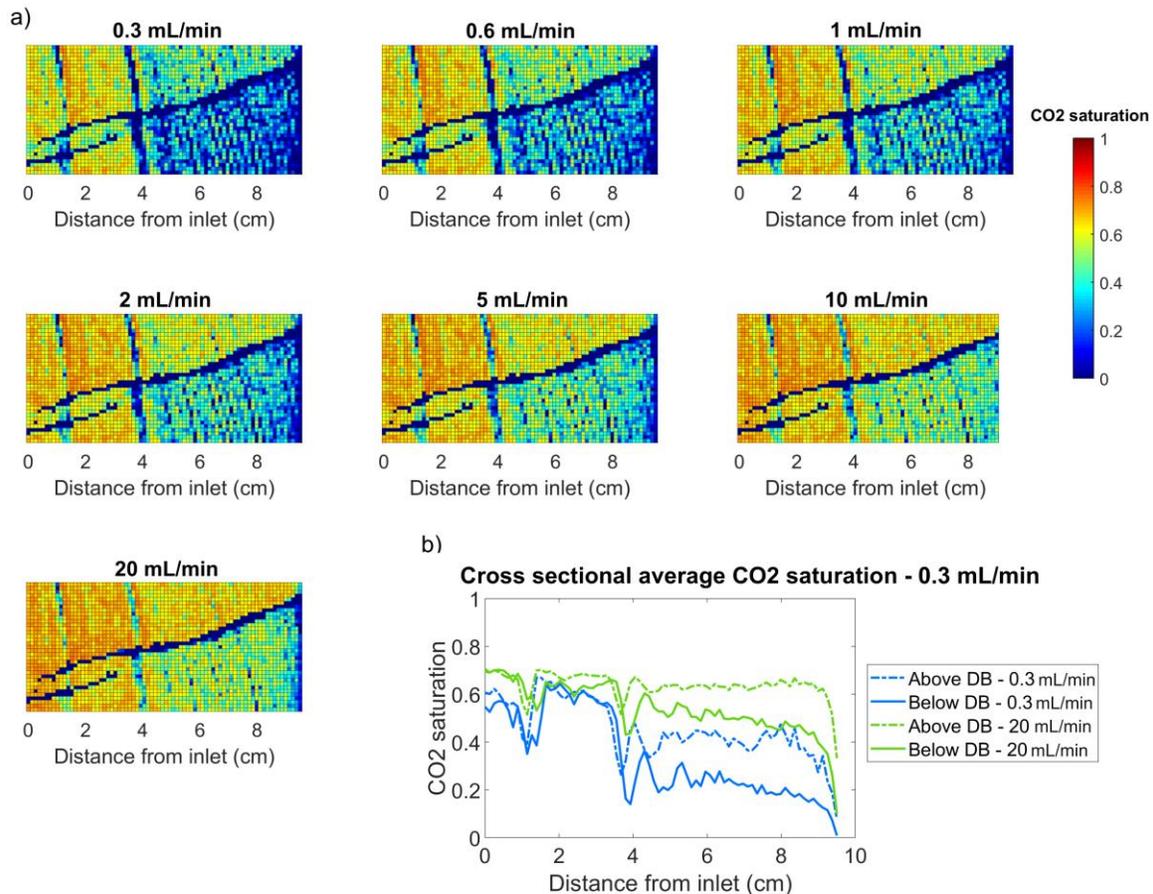
384 **4 Numerical modeling of multiphase flow experiments**

385 Multiphase fluid flow simulations were conducted using the GPRS simulator to fully understand
386 the CO₂ saturation distribution and migration in the presence of deformation bands. The porosity
387 and permeability fields used in the model were those derived in section 3.2 and 3.3. The capillary
388 entry pressure was calculated for each grid block in the model using the Leverett J-function model,
389 which scales the capillary pressure curve derived from the experimental data based on the porosity
390 and permeability distribution (Li, 2011). Water and CO₂ relative permeability curves were
391 calculated using the Brooks-Corey model (Brooks & Corey, 1964). Details of input parameters are
392 included in supporting information (Text S2, Figure S3, S4, S5, Table S2). Given that the bands
393 traverse the full core width, for simplicity, a 2D model was developed (grid size 35X78 cells, pixel
394 resolution 0.125 cm) to model the central rectangular cross-section along the core. The model is
395 initially fully saturated with water prior to injection of CO₂. Boundary conditions (Figure S6 in
396 supporting information) were no flow conditions on the lateral faces, a time-varying CO₂ flow
397 rate, adjusted for cross-sectional area, at the inlet face equal to the experimental flow rate (Figure
398 6a) and a fixed outlet pressure of 9 MPa.

399 *4.1 Multiphase fluid flow simulation with capillary end effect*

400 In the experimental setup there is a small gap between the core and the outlet cap, which effectively
401 creates a reservoir at the end of the core where the permeability and porosity are very high. This
402 zone creates a capillary pressure discontinuity. A negative gradient of CO₂ saturation (Pini &
403 Benson, 2013) is associated with this “discontinuity of capillarity in the wetting phase” (Huang &
404 Honarpour, 1998), creating a so-called capillary end effect. To simulate this effect, a small
405 reservoir characterized by low capillary entry pressure (0.02 kPa), high porosity (0.7), and high
406 permeability (100000 mD) was placed in the final right-hand column of grid cells at the end of the
407 model.

408 Simulation results show, for all flow rates, a lower CO₂ saturation in the compartment below the
409 deformation bands than the one above it (Figure 7a). A decreasing CO₂ saturation near the end of
410 the core is also apparent (Figure 7b). As in the experiment, the difference in saturation above and
411 below the bands is higher toward the outlet of the core.



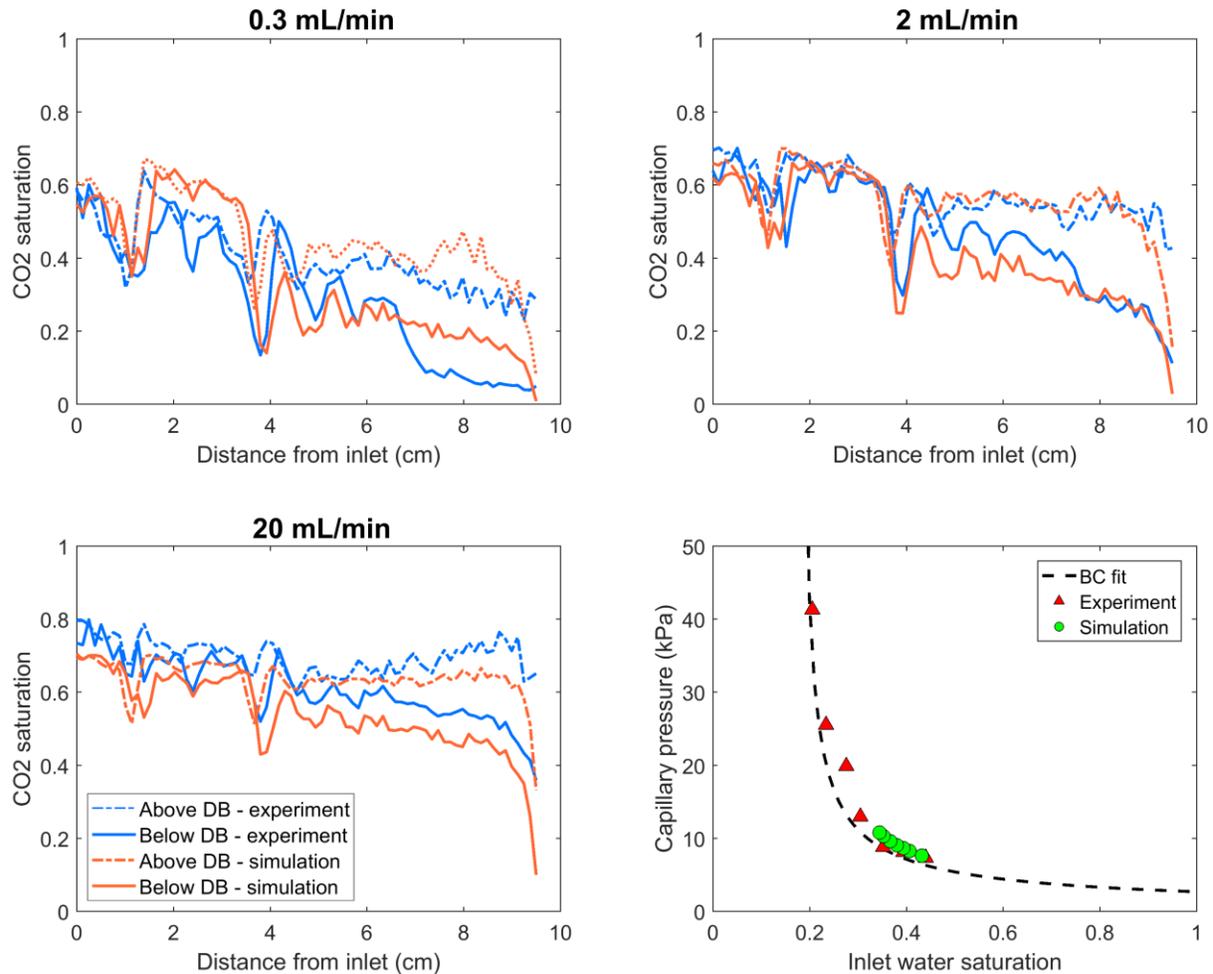
412

413 **Figure 7.** a) Simulation results for the model with small reservoir at the end (capillary end effect).
 414 Lower CO₂ saturation is seen in the portion below the deformation bands. b) Comparison between
 415 the two compartments at 0.3 mL/min and 20 mL/min. This plot illustrates the negative CO₂
 416 saturation trend due to capillary end effect. For all the flow rates, there is a lower CO₂ saturation
 417 in the compartment below the bands compared to above the bands.

418 The model is able to capture the main characteristics of the experiment, specifically the difference
 419 in saturation between the two compartments and the effect of the laminae on CO₂ distribution
 420 (Figure 8). At 0.3 mL/min, the model over-predicts the CO₂ saturation towards the outlet (Figure
 421 8 top left). This is likely related to an underestimation in the model of the capillary entry pressure
 422 near the outlet. As the viscous pressure drop increases with increasing flow rate, the influence of
 423 capillary heterogeneities on fluid saturation distribution decreases. At 2 mL/min (Figure 8 top
 424 right) the model agrees with the experimental CO₂ saturation at the outlet of the core, suggesting
 425 that the decreasing CO₂ saturation trend in both compartments is strongly influenced by the
 426 capillary end effect. At 20 mL/min the model under-predicts the final CO₂ saturation (Figure 8
 427 bottom left). This can be explained by the fact that, during experiments, the capillary end effect
 428 has lower extension at high flow rates (Guédon, et al., 2017).

429 For flow rates higher than 1 ml/min, the simulation results show higher inlet water saturation and
 430 therefore lower capillary pressure values as compared to the experimental results (Figure 8 bottom

431 right). This is probably due to either an overestimation in the model of the capillary entry pressure
 432 near the inlet of the core or small errors in the relative permeability used within the model.



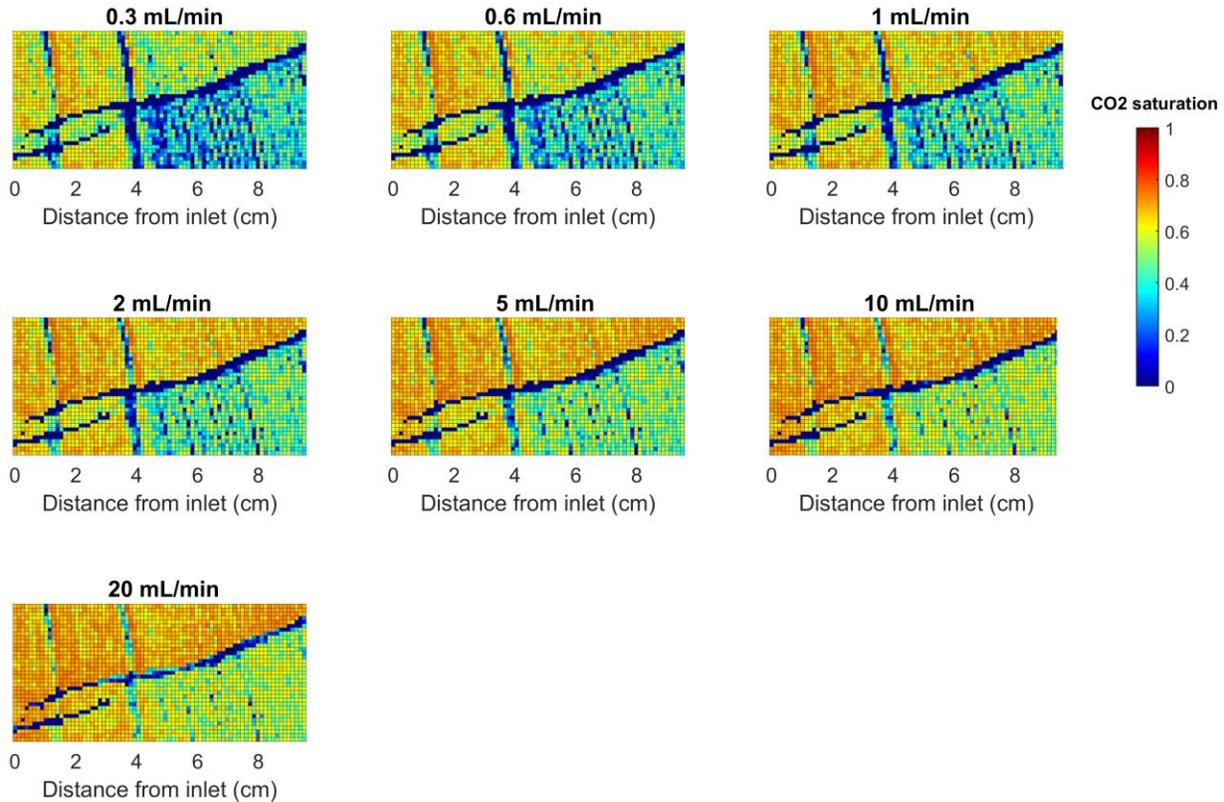
433

434 **Figure 8.** Comparison between experimental (blue) and simulation results (orange) for three
 435 different flow rates. The model captures the CO₂ saturation behavior in the experiment at 0.3
 436 mL/min (upper left) and 2 mL/min (upper right). At 0.3 mL/min, the saturation shadow zone seen
 437 in the experiment is not replicated in the simulation. At 20 mL/min (lower left) the negative trend
 438 shown in the simulation is not representative of the experimental results. (lower right) Inlet
 439 capillary pressure values for all flow rates, resulting from experiments and simulations with small
 440 reservoir at the end of the core. The capillary pressure in steady state conditions can be assumed
 441 to be equal to the differential pressure measured at the inlet slice of the core (Pini, et al., 2012).

442 4.2 Multiphase fluid flow simulation without the capillary end effect

443 To exclude the influence of the capillary end effect on the CO₂ saturation distribution, and isolate
 444 the impact of the deformation bands, the model was repeated with no small reservoir at the end.
 445 Results (Figure 9) show that the deformation bands continue to compartmentalize fluids in the host
 446 rock and that the compartment below the bands continues to have a lower saturation than the one
 447 above. At 20 mL/min small portions of deformation bands become saturated with CO₂, leading to

448 cross flow between compartments above and below the bands. As shown in Figures 2, 5 and S5,
 449 there is no substantial difference in porosity, absolute permeability or capillary entry pressure
 450 between the two compartments. As is the case with single phase flow, the difference in CO₂
 451 saturation can be attributed to the geometry of the two compartments. The compartment above the
 452 bands has a smaller cross-sectional area towards the outlet, resulting in a higher fluid velocity and
 453 a higher pressure gradient when compared to the compartment below the bands.



454

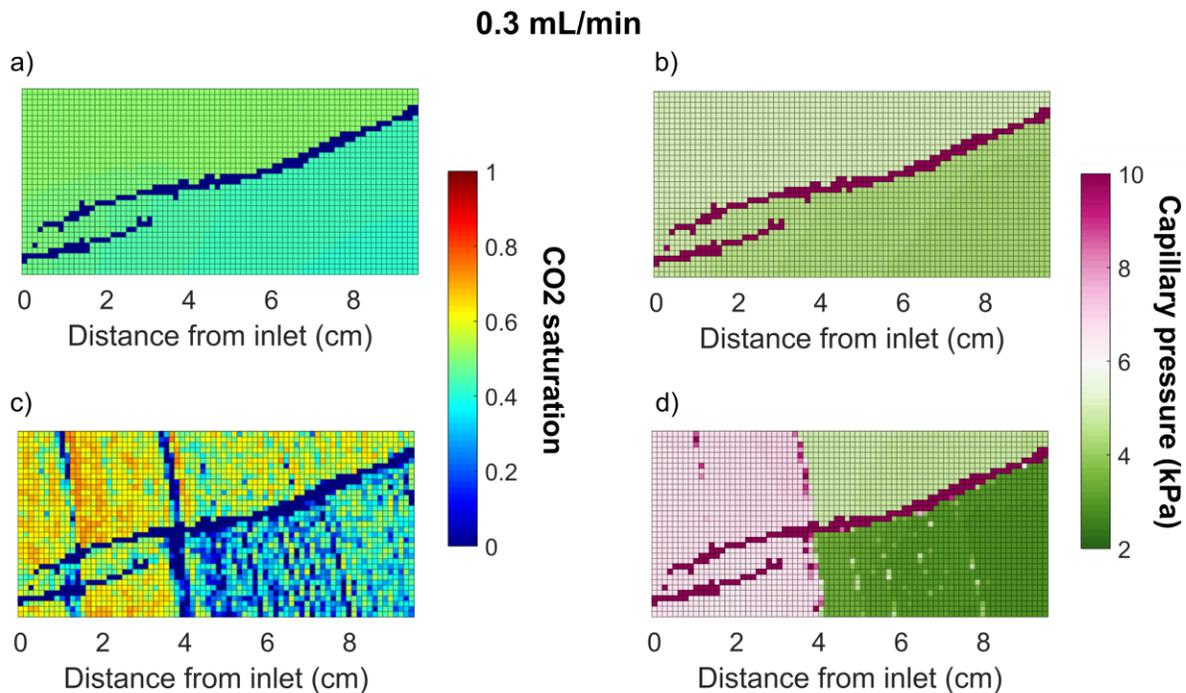
455 **Figure 9.** Simulation results for the model without small reservoir at the end (with no capillary
 456 end effect). Lower CO₂ saturation is shown in the compartment below the deformation bands.
 457 Some portions of the deformation bands are partially saturated with CO₂ at 20 mL/min.

458 *4.3 Multiphase fluid flow simulation without laminae*

459 The experimental observations (Figure 6) show that the laminae have a significant influence on
 460 CO₂ migration. To distinguish the relative effects on CO₂ saturation of the deformation bands and
 461 the laminae, a simulation was conducted with no end effects and with the laminae removed.

462 Figure 10 shows CO₂ saturation and capillary pressure distribution with and without the laminae
 463 for an injection rate of 0.3 mL/min. This flow rate has been chosen, because the highest influence
 464 of laminae on fluid flow has been observed during these drainage flow conditions. With the
 465 laminae removed, the difference between the CO₂ saturation above and below the bands is less
 466 pronounced; the low saturation levels in the bottom host rock compartment are maintained at the
 467 inlet. These results confirm the earlier experimental interpretation that CO₂ saturation increases

468 upstream of the laminae. This demonstrates that the laminae act as capillary barriers at low flow
 469 rates.



470

471 **Figure 10.** a) CO₂ saturation for the model without end effect and laminae. b) Capillary pressure
 472 calculated for the model without end effect and laminae. c) CO₂ saturation for the model of the
 473 core without end effect. d) Capillary pressure calculated for the model of the core without end
 474 effect. The presence of laminae increases both saturation and capillary pressure for the first 4 cm
 475 of the core.

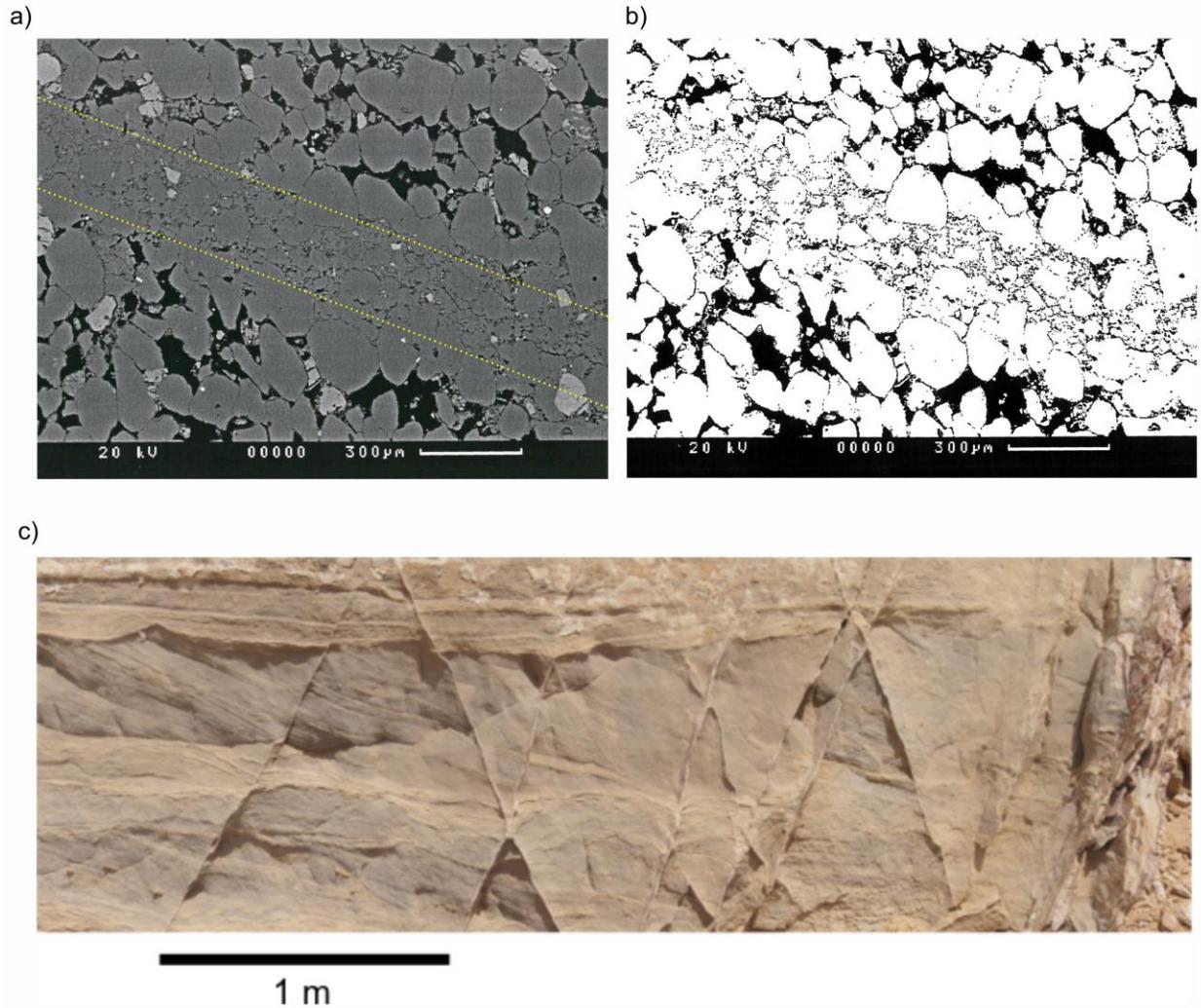
476 **5 Discussion**

477 The effect of cataclastic deformation bands on single and multiphase fluid flow have been
 478 investigated *in situ* for the first time. While deformation bands do not entirely surround any
 479 individual portion of the host rock in our core sample, we find that they significantly contribute to
 480 fluid compartmentalization. Deformation bands subdivide the host rock into two distinct regions,
 481 above and below the deformation bands. The compartmentalization results in differing fluid
 482 velocity distributions and CO₂ saturation values. The low permeability of the bands, demonstrated
 483 by the single phase flow experiments, together with their high capillary entry pressure,
 484 significantly inhibit cross-flow of CO₂ between the two compartments.

485 In our experiments, the deformation bands are sub-parallel to the flow direction and therefore fluid
 486 is not forced to travel across them. This results in the deformation bands remaining almost entirely
 487 unsaturated with CO₂ and almost no cross-flow occurring. If the deformation bands were oriented
 488 perpendicular to the flow, we would expect a different outcome. The grain size distribution within
 489 individual laminae is narrow because the Navajo sandstone is aeolian. However, within the
 490 deformation bands the particle size distribution is much broader. Figure 11a shows a microscale

491 image of a deformation band from the Big Hole fault field site. The band is a mixture of larger
492 ‘survivor’ grains and very fine crushed grain material. This results in almost no residual porosity,
493 since the crushed material entirely fills the gaps between the larger grains (Figure 11b). With
494 deformation bands perpendicular to the flow we would expect an effect similar to that of the finer-
495 grained laminae, but much more pronounced as the entry pressure will be much higher.

496 To understand the implications of our research for multiphase fluid injection at a commercial scale,
497 it is important to be able to characterize deformation band frequency and orientation within a
498 reservoir. Deformation bands do not generally occur with a unique orientation, or indeed, as single
499 isolated bands; they form conjugate sets (Figure 11c) and are often present in thick anastomosing
500 clusters. This implies a high degree of 3D reservoir anisotropy and the potential for significant
501 CO₂ channeling in lozenge-shaped compartments confined by deformation bands. Lower fluid
502 saturation zones (shadow zones), fluid compartmentalization, injection pressure buildup and
503 preferential channels for fluid migration, are all potential effects of the presence of deformation
504 bands in a sandstone reservoir. Consequently, adequate characterization of petrophysical
505 deformation band properties, through micro-structural analysis or flow experiments, alongside
506 their orientation, thickness, and spatial distribution, through scan-line sampling, well logs and
507 borehole seismic data, are all important factors to consider when estimating the likely storage
508 volume and injection pressure of, for example, a potential CO₂ storage reservoir.



509

510 **Figure 11.** a) BSEM of a deformation band in the Navajo sandstone at the Big Hole Fault.
 511 Deformation bands is included in the yellow dashed lines; pores are in black. b) Segmented image
 512 of Figure 11a. Smaller grains (white) and pore space (black) along the band. c) Conjugate sets of
 513 deformation bands from an outcrop of the Slick Rock Member of Entrada Sandstone in Utah.

514 **6 Conclusions**

515 Single phase and multiphase core flooding experiments were conducted in a sandstone core
 516 presenting diagonal cataclastic deformation bands and two lower-porosity laminae. In the single
 517 phase experiment, PET imaging revealed that the presence of the diagonal deformation bands
 518 created a strong difference in the velocity distributions between compartments of the host rock
 519 above and below the deformation bands. This difference was not caused by any difference in
 520 porosity and permeability between the two compartments, but instead was attributed to the
 521 geometry of the band. No effect of the laminae on single phase flow transport was apparent.

522 High-pressure CO₂ injection drainage experiments were conducted in the same core and imaged
 523 with a medical X-ray CT scanner, allowing progressive imaging of CO₂ saturation at different flow

524 rate conditions. Results show that both the finer-grained laminae and the deformation bands acted
525 as capillary barriers. The laminae form weaker capillary barriers than the deformation bands, with
526 the compartment below the bands presenting lower CO₂ saturation for all flow rates, particularly
527 toward the outlet. Numerical simulations of the experiments at low flow rates revealed that while
528 some of the low saturation at the outlet was due to the experimental capillary end effect simulations
529 without the end effect also predicted significant differences in CO₂ saturation due to the presence
530 of the bands. Deformation bands have extremely low permeability and porosity, and a very high
531 capillary entry pressure that inhibits CO₂ migration across the bands. The bands remained saturated
532 with water during the experiments, contributing to the isolation of the two host rock compartments.

533 At the reservoir scale, deformation bands form conjugate sets and are often present in thick
534 anastomosing clusters. Thus, deformation bands have the potential to channel and
535 compartmentalize both single and multiphase fluid flow. These findings have important
536 consequences for predicting multiphase flow in sandstone reservoirs and specific implications for
537 storage capacity and injectivity of carbon and storage in geological formation.

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