- 1 Fault seal modelling the influence of fluid
- ² properties on fault sealing capacity in hydrocarbon

3 and CO₂ systems

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- 15 Keywords: fault seal; hydrocarbons; CO₂; interfacial tension; wettability; contact
- 16 angle; fluid properties; Otway Basin.
- 17 Abstract
- 18 Fault seal analysis is a key part of understanding the hydrocarbon trapping
- 19 mechanisms in the petroleum industry. Fault seal research has also been expanded
- 20 to CO₂-brine systems for the application to Carbon Capture and Storage (CCS). The
- 21 wetting properties of rock-forming minerals in the presence of hydrocarbons or CO₂
- are a source of uncertainty in the calculations of capillary threshold pressure, which
- 23 defines the fault sealing capacity. Here we explore this uncertainty in a comparison
- 24 study between two fault-sealed fields located in the Otway Basin, south-east
- 25 Australia. The Katnook field in the Penola Trough is a methane field, while Boggy
- 26 Creek in Port Campbell contains a high-CO₂/methane mixture. Two industry
- 27 standard fault seal modelling methods (Yielding et al., 2010; Sperrevik et al., 2002)

28 are used to discuss their relative strengths and applicability to the CO₂ storage 29 context. We identify a range of interfacial tensions and contact angle values in the 30 hydrocarbon-water system under the conditions assumed by the Yielding et al. 31 (2010) method. Based on this, the uncertainty related to the spread in fluid 32 properties was determined to be 24% of the calculated threshold capillary pressure 33 value. We propose a methodology of threshold capillary pressure conversion from 34 hydrocarbon-brine to the CO₂-brine system, using an input of appropriate interfacial 35 tension and contact angle under reservoir conditions. The method can be used for any fluid system where fluid properties are defined by these two parameters. 36

37 1 Introduction

38 Faults can be either pathways for, or barriers to fluid migration in the 39 subsurface and to the surface. Fault seal analytical techniques have been 40 developed to improve the prediction of hydrocarbon traps suitable for exploration. 41 More recently, fault seal research has expanded to applications to Carbon Capture 42 and Storage (CCS), where faults can act to: decrease the maximum storage 43 capacity of the reservoir; become unwanted barriers to fluid migration along the 44 planned injection pathway, causing pressure increase and limiting the maximum rate 45 of injection; or, provide a conduit for leakage of CO₂.

46 Two distinct methodologies of predictive modelling of the threshold capillary 47 pressure, which is a proxy for fault sealing capacity to hydrocarbons, have been 48 developed in the last two decades: one based on a calibration of a global dataset of 49 known sealing faults (Bretan et al., 2003; Yielding et al., 2010), and another, based 50 on laboratory measurements of fault samples (Sperrevik et al., 2002). Both of these 51 techniques have been widely applied to hydrocarbon systems. Fault capacity to seal 52 for CO_2 has been explored in theoretical studies (Iglauer, 2018; Miocic et al., 2019; 53 Naylor et al., 2010), yet there have been few attempts to test the methodology with 54 real geological examples (Bretan, 2016; Bretan et al., 2011; Yielding et al., 2011).

In terms of practically applying model results to either exploration of hydrocarbons or CO₂ sequestration, the subject of interest is not the exact threshold capillary pressure of a certain fault but rather the implications of that value to the desired industrial activity. In exploration, this is applied to estimate maximum column height and determine the economic viability of production. It is therefore important to

estimate how the uncertainty associated with the predictive method impacts the
prospect. In the context of CO₂ storage, threshold capillary pressure is used to
define the reservoir storage capacity. In this case the aim is not to overpressure the
fault and thus cause leakage. The practical use of fault seal modelling therefore
requires a good understanding of the uncertainty associated with the two different
approaches.

66 The interfacial tension (IFT) and the contact angle (CA) are the main fluid-67 specific properties controlling the capillary seal and the key parameters used in both 68 hydrocarbon and CO₂ studies. The wetting properties of various rock-forming minerals are different for CO₂ and hydrocarbons, which has caused a concern that 69 70 the seal rocks proven to retain hydrocarbon columns might be less sealing to CO₂ 71 (Chiquet et al., 2007b; Daniel and Kaldi, 2009; Guariguata-Rojas and Underhill, 72 2017; Tenthorey et al., 2014). A recent study by Miocic et al. (2019) explored the 73 interplay between uncertainties in CA, IFT and fault rock composition in the CO₂-74 brine system. The results highlighted that higher phyllosilicate content in the fault 75 rock reduces the threshold capillary pressure in the CO₂-brine system due to the 76 wettability of the clay minerals in the presence of CO_2 , especially at depths > 1 km.

Our understanding of CA and IFT primarily relies on empirical measurements,
meaning that significant uncertainty exists in both hydrocarbon and CO₂-brine
systems. While the above concerns are valid for the CO₂ storage, the existing
uncertainties associated with CA and IFT also exist in the hydrocarbons. This is
because of the wide range of chemical compositions of crude oil and the difficulty of
sampling undegassed reservoir fluids.

83 In this contribution we investigate the uncertainty associated with the fluid 84 properties (CA, IFT) as well as geological assumptions required for the model (depth 85 at the time of faulting and maximum burial depth) in two field examples. One, 86 methane gas field in South Australia (Katnook), and another, a high CO₂/methane 87 mixture in Port Campbell, Victoria (Boggy Creek). In both cases, a gas column is 88 supported by the fault rock and the column height is known. The fields are located in 89 the Otway Basin, which is very well characterised in respect to hydrocarbon exploration as well as CO₂ storage. These case studies therefore provide a realistic 90 91 example of the level of uncertainties that can be expected in future potential CO₂ 92 storage sites.

93 This approach allows us to verify if the model predictions are valid and 94 systematically compare the uncertainties in the CO₂ and methane system. Fault seal 95 analysis is performed using the Sperrevik et al. (2002) and Yielding et al. (2010) 96 fault seal modelling methods, discussing the differences in the modelling 97 approaches, their associated uncertainties and suitability for the CO₂-brine system. 98 The former method inherently allows the conversion from mercury-air system to 99 CO₂-brine, while the latter method is calibrated to a hydrocarbon system. We 100 summarise the current understanding of the IFT and CA ranges in hydrocarbons 101 that the Yielding et al. (2010) method is based on to define the expected IFT and CA 102 distribution and their mean values. Based on this, we propose a new calibration of 103 the Yielding et al. (2010) algorithm to the CO₂-brine system.

104 2 Fault rock seal dependencies

105 Fault rock seals occur when movement along a fault plane creates a low-106 permeability fault rock, and depend on the fault rock composition as well as the 107 properties of the fluids in the system. In siliciclastic sand-shale sequences, the 108 sealing fault rocks are characterised by continuous clay-rich smears (Lindsay et al., 109 1993). Their thickness is favoured by greater thickness of shale beds in host rocks, 110 weight of the overburden, and burial depth (Lehner and Pilaar, 1997). Quartz 111 cementation at temperatures above 90 °C or ~>3 km further decreases fault rock 112 porosity and increases the sealing potential (Fisher and Knipe, 1998; Rimstidt and 113 Barnes, 1980). The resulting fault rock may act as baffle to fluid migration through a 114 process of capillary sealing, which is created by the opposing forces between the 115 two phases at their interface - the wetting phase (water or brine) and the non-116 wetting phase (hydrocarbons or CO₂, in this context) (Fisher and Knipe, 1998; Watts, 117 1987; Yielding et al., 1997). Capillary seals fail when the fluid buoyancy pressure 118 exceeds the threshold capillary pressure. Capillary threshold pressure (P_c) is 119 therefore a key fault rock attribute used in the hydrocarbon exploration industry to 120 determine the sealing potential of the fault and calculate maximum column heights 121 (h_{max}) , using the relationship between the height of the fluid column and the 122 buoyancy pressure it exerts on the sealing rocks (Schowalter, 1974):

123
$$P_c = \frac{2IFT \times cos\theta}{r}$$
(1)

124
$$h_{max} = \frac{P_c}{(\rho_h - \rho_w)g}$$

125 Where IFT is the interfacial tension between the fluids, θ is the contact angle, 126 r is the effective pore throat radius, ρ is density, g is acceleration due to gravity, h 127 and w denote hydrocarbons and water.

(2)

128 The interfacial tension and contact angle (or wettability) are the key 129 properties controlling capillary seal and depend on many factors including pressure, 130 temperature, fluid type, fluid density and rock mineralogy (e.g. Iglauer et al., 2015; 131 Nordgard Bolas et al., 2005; Øren and Bakke, 2003; Radke et al., 1992; Schowalter, 132 1974). The influence of these factors is a key concern in describing fault zone 133 behaviour. The advantage, however, is that the characteristics of fluids and their 134 affinity to reservoir rock can be approximated by these two input parameters, and 135 therefore applied in the same manner to systems involving hydrocarbons, CO_2 or 136 any other fluid type of interest.

137 The buoyancy pressure exerted on the fault rock by the column of fluid is 138 greater with increasing density contrast between the wetting and the non-wetting 139 phases. Under typical reservoir conditions, density of methane ranges between 100 140 -300 kg/m³, CO₂ is approximately 400 -600 kg/m³ and oil density varies between 141 700 – 1000 kg/m³ (Danesh, 1998). Brine density depends on salinity and has a 142 value of 1000-1150 kg/m³. It is therefore apparent, that a fault rock with a certain 143 capillary threshold pressure would retain a smaller column of methane than of CO₂ 144 or oil, if the other parameters were the same. However, the differences in interfacial 145 tension and CA between CO₂ and hydrocarbons also impact the threshold capillary 146 pressure of the fault rock in a CO₂-brine system (Chiquet et al., 2007b). The 147 interplay between IFT, CA and fluid density therefore is key to consider in applying 148 fault seal modelling techniques to CO₂ sequestration.

The effective pore throat radius of a fault zone is impossible to directly determine, and by standard practice is approximated using a predictive algorithm based on the clay content of the faulted rocks, such as SGR (Yielding et al., 1997). Two different approaches have been developed to link SGR to capillary threshold pressure. One approach is based on laboratory experiments of mercury-air injection tests in micro-fault samples and subsequent correlation of measured capillary

155 pressures to sample clay content (Sperrevik et al., 2002), based on earlier studies 156 by Knipe (1997), Gibson (1998). The second approach uses data from known hydrocarbon traps sealed by faults to empirically correlate the maximum observed 157 158 buoyancy pressures (assumed equivalent to threshold pressure) to SGR values 159 (Bretan et al., 2003; Yielding, 2002; Yielding et al., 2010). The two approaches have 160 been termed 'deterministic' and 'empirical' respectively (Yielding et al., 2010), and 161 will be referred to as such in the forthcoming text. The two methods are often used 162 in conjunction and have been shown to produce similar results in certain but not all 163 SGR/burial depth configurations (Yielding et al., 2010). To date, the application of 164 these methods to the CO₂-brine systems has been limited (Bretan et al., 2011).

165 The deterministic approach is based on laboratory measurements of fault 166 rock permeability from a variety of fault structures within reservoir core samples and 167 requires a conversion from the mercury-air system to hydrocarbon-water or CO2-168 brine system by using appropriate values for IFT and contact angle between the 169 fluid and the wetting phase (Sperrevik et al., 2002). In contrast, the empirical 170 approach (Bretan et al., 2003; Yielding, 2002) is based on a calibration of SGR 171 values and across-fault buoyancy pressure differences of known sealing faults. 172 Importantly, the calibration includes only hydrocarbons at depths greater than 1.5 173 km. This means that theoretically, the method can only be applied to fluid systems 174 which fall within the range of IFT and contact angle parameters as the hydrocarbon 175 field used in the calibration. Further constraining this range is discussed below 176 before we propose a methodology to convert fault seal modelling results from 177 hydrocarbons to CO₂-brine system.

179 **3 Geological background**

In this study we describe two gas fields in the Otway Basin, Victoria, Australia: The
Katnook field in the Penola Trough and the Boggy Creek field in the Port Campbell
embayment. Below we outline the geology of the fields in terms of stratigraphy, trap
geometries and gas charge.

184 3.1 Basin stratigraphy

185 The present day geometry of the Otway Basin was developed during the 186 Cretaceous to Miocene rifting with a period of inversion in the mid-Cretaceous, when 187 the rift axis moved south (Teasdale et al., 2003). A series of graben and half-graben 188 structures consist of compartmentalised fault-bound reservoirs, with numerous 189 hydrocarbon and CO₂ accumulations (Fig. 1). Two case studies discussed here present examples of gas column retention by a fault rock in a situation of reservoir-190 191 reservoir juxtaposition. Katnook in the Penola Trough is a methane field, while the 192 Boggy Creek field in Port Campbell contains a high-CO₂/methane mixture.

193 The two fields are within different reservoir formations at different 194 stratigraphic intervals (Fig. 1). The Katnook field is stratigraphically lower, located in 195 Pretty Hill Formation of 2 - 4.5 km thickness, within the Pretty Hill Sandstone. The 196 main target reservoir is the Pretty Hill Sandstone member at the top of the sequence 197 (Lyon et al., 2005). The formation consists of massive, slumped and cross-bedded 198 sand packages, classified as lith-arenites to feldspathic lith-arenites (Little and 199 Phillips, 1995). The Laira Formation forms a regional seal, comprised of siltstones 200 and shales interbedded with sandstones. The Katnook sandstone at the top of the 201 Crayfish Group (consisting of both the reservoir and the seal lithologies) is also gas-202 bearing, but is not a subject to this discussion. Katnook-1 and 2 are production wells 203 targeting Katnook sandstone within the Crayfish Group, while Katnook-3 produces 204 from the deeper Pretty Hill Formation. Shale units within the lower parts of the Pretty 205 Hill Formation and the underlying Casterton Formation are the oil and gas source 206 rocks in the Penola Trough and the SW part of the basin (Boreham et al., 2004).

- 207 The Boggy Creek CO₂ field is stratigraphically higher, within the Waarre 208 Sandstone, comprised of interbedded siltstones and shales, segregated into four 209 units defined by depositional environments. Unit C, the main reservoir interval, is 210 poorly sorted, medium to coarse-grained quartz arenite (Watson et al., 2004). The 211 underlying Eumeralla Formation consist of inter-bedded lithic sandstones, siltstones, 212 coals and claystones (Cockshell et al., 1995). The deeper coal-rich units of 213 Eumeralla Formation are the source rocks in the SE part of the basin. The Belfast 214 Mudstone overlies the reservoir and forms a regional seal (Boreham et al., 2004).
- The Waarre sandstone is approx. 90 m thick and the main producing interval
- within it (Unit C) is 25 -40 m thick (Dance, 2013). The underlying Eumeralla
- 217 Formation is up to 3 km thick (Cockshell et al., 1995). Significant oil shows have
- 218 been observed within the Eumeralla Formation in other parts of the basin (Lisk,
- 219 2004) and therefore good connectivity between the Waare and Eumeralla units is
- 220 expected despite the silt and clay inter-beds.

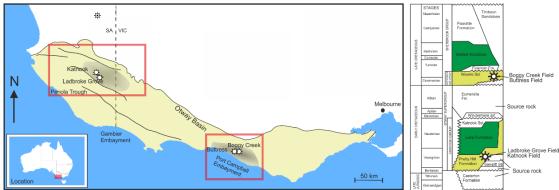


Figure 1. Location map of Penola Trough (Katnook/Ladbroke Grove fields) and Port
Campbell (Buttress/Boggy Creek fields). Both localities are within the Otway Basin. Inset on
the right shows the location of both reservoirs within the stratigraphic column (adapted from
Lyon et al., 2004).

- 3.2 Trap geometry
- 228 The Katnook field is bound by the Katnook fault to the north and Ladbroke
- Grove fault to the south (Fig. 2a). The northern side of the field is juxtaposition-
- 230 sealed against Crayfish Group shales, while the southern side reaches the Ladbroke
- 231 Grove Fault, where the reservoir is self-juxtaposed (Fig. 2c). The Boggy Creek field
- is bound by the Boggy Creek Fault to the south and the Buttress Fault to the north

- 233 (Fig. 2b). Similarly to the Katnook field, the main seal to the reservoir is provided by
- juxtaposition seal to the south, but fault rock seal exists to the north (Fig. 2d).

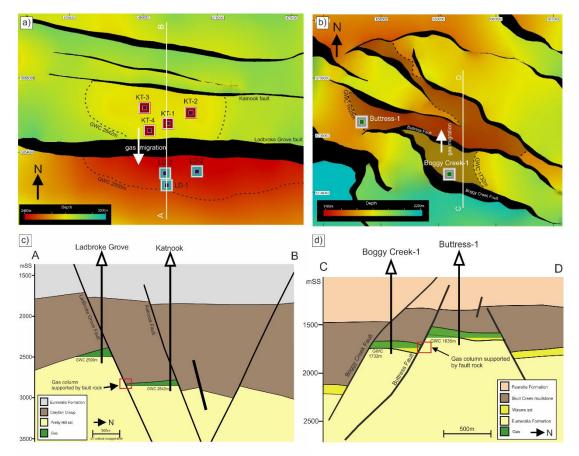


Figure 2. Map and cross-sectional views of Penola Trough (a, c) and Port Campbell (c, d) 237 gas field locations. a) Map view of the top of the Pretty Hill reservoir horizon, coloured by 238 depth. b) Map view of the top of the Waarre sandstone reservoir horizon, coloured by depth. 239 c) Cross-section view of line A-B from figure (a). Ladbroke Grove and Katnook fields in 240 Penola Trough. Cross-section drawn from seismic data using 3x vertical exaggeration. 241 Katnook field is supported by Katnook fault to the north (juxtaposition seal) and Ladbroke 242 Grove fault to the south (fault rock seal). d) C-D cross-section view (from figure b) of the 243 Boggy Creek and Buttress fields in Port Campbell. Cross-section drawn from seismic data 244 without vertical exaggeration. Boggy Creek gas field is retained by juxtaposition seal to the 245 south and fault rock seal to the north. The adjacent Buttress field is structurally higher. 246

247

248 3.3 The sequence of gas charge events

The two main phases of hydrocarbon generation in the Otway Basin are estimated at mid-Cretaceous (Boult et al., 2004) and mid-Paleogene (Duddy, 1997), based on thermal maturation modelling and the relationship between GWC positions above spill points and known gas diffusion rates (Lyon et al., 2005). Early oil/wet gas charge was flushed or diluted by later dry gas charge (Boreham et al., 2004). Methane charge was followed by a later stage magmatic CO₂ injection (Chivas et al.,
1987; Lyon et al., 2005; Watson et al., 2003). Due to the sealing or partially sealing
nature of bounding faults, the CO₂/methane ratio significantly varies across
geographically closely located fields.

258 The Ladbroke Grove field contains CO₂, with higher concentrations at the 259 base (49%) and lower at the top of the reservoir interval (27%). The Katnook field 260 contains primarily methane with only trace amounts of CO_2 (0.2%). ³He/⁴He, 261 CO₂/³He and neon isotopic ratios indicate that CO₂ in Ladbroke Grove is of mantle 262 origin (${}^{3}\text{He}/{}^{4}\text{He} = 1.46 \text{ R/R}_{\text{A}}$) (Karolytė, 2018). ${}^{3}\text{He}/{}^{4}\text{He}$ ratios in the Katnook field are 263 slightly elevated above the crustal values (0.06 R/ R_A), but any mantle-sourced noble 264 gases are decoupled from the migrating CO₂ (Karolyte, 2018). These geochemistry 265 results suggest that methane has likely migrated through the fault rock from Katnook 266 to the Ladbroke Grove field, while the later CO₂ charge was restricted to Ladbroke 267 Grove only.

268 The Boggy Creek and Buttress fields both contain mixtures of mantle CO₂ 269 and methane. CO₂ concentrations within the traps increase with depth because of 270 its higher density, and Boggy Creek (87% CO₂) is more CO₂-rich than Buttress (77% 271 CO₂) (Karolyte et al., 2019). While independent charge to both fields cannot be 272 completely excluded, the observed concentration gradient suggests that CO_2 was 273 first charged to the Boggy Creek field, and later migrated to Buttress. The trap is not 274 filled up to the spill point, suggesting this migration occurred through the fault rock 275 which supports the column.

276

4 Methods

4.1 Geological 3D models

This work has been undertaken using a compilation of existing industry and
academic datasets. 3D model development, structural and fault seal analysis was
undertaken using TrapTester[™] software. The Penola Trough 3D model was
developed by Paul Lyon and published in Lyon et al. (2005b, 2007, 2004). It was
constructed by interpretation of the 3D Balnaves-Haselgrove seismic survey in time

and pseudo-depth (Lyon et al., 2004). The 3D model used for Port Campbell area
was developed by Ziesch et al. (2017) using a combination of OGF93A, ONH01 and
Curdie Vale 3D seismic surveys. Seismic data reinterpretation in this study has led
to addition of some new faults and modification of fault and horizon geometries in
the original models.

289 4.1.1 **V-shale**

290 The V-shale curves for the studied wells were created from GR wireline logs. 291 'Clean sand' and 'pure shale' (0 and 100% V-shale) values were determined by 292 correlating GR measurements to core descriptions and, where possible, core 293 permeability tests from the well completion reports. The Waarre sandstone is 294 feldspathic (Watson et al., 2003), which is reflected in the relatively high chosen API 295 (American Petroleum Institute unit) values of clean sands. The strength of the GR 296 signal is often not uniform between different wells, in which case different clean 297 sand and pure shale values have to be chosen to produce internally consistent V-298 shale logs. The V-shale values were calculated using the linear response equation 299 (Asquith et al., 2004):

$$300 V_{Shale} = I_{GR} = \frac{GR_{log} - GR_{sand}}{GR_{shale} - GR_{sand}} (3)$$

302

4.1.2 Fault seal modelling

The intersection lines between the top of the reservoir formation on the footwall and the hanging wall side of the fault were created on the fault planes (e.g. Yielding & Freeman, 2016). Manual quality check techniques such as projecting seismic slices on the fault plane were used to accurately map out the geometry of the intersections. Allan diagrams (Allan, 1989) were created to identify the areas of interest where reservoir formation is juxtaposed against another permeable rock on the other side of the fault.

310 Buoyancy pressure is calculated on the 3D surface of the fault based on the 311 input of gas and water pressure gradient and the gas water contact (GWC). This 312 data was obtained from repeat formation tester (RFT) plots in well completion 313 reports (WCRs) from Buttress and Ladbroke Grove fields. Pressure profile data did 314 not exist for Katnook and Boggy Creek fields, so gas pressure gradients were 315 calculated from gas densities. Gas densities at reservoir conditions were calculated 316 using the Peng-Robinson equation of state (Peng and Robinson, 1976). A summary 317 of input parameters relevant to buoyancy pressure calculation is given in Table 1.

Table 1. Summary of parameters used in the buoyancy pressure calculations. Temperature and pressure relevant where density was calculated using equation of state rather than obtained from RFT measurements. Major gas compositions are from Karolytė (2018) and Karolytė et al. (2019).

Field	Temperature °C	Pressure MPa	GWC mSS	<mark>Բ</mark> ա kg/m³	ዖ _g kg/m³	Major gas 323 composition			
						C₁+	N ₂	c <u>32</u> 4	
Penola Trough									
Ladbroke Grove	104	23	2500	927	244	45	7.2	325	
Katnook	118	28	2842	1035	125	97	3.2	<u>32</u> 6	GR
Port Campbell								327	was
Buttress	62	16	1635	1035	382	22	1.9	3 ⁷⁷ 328	calc
Boggy Creek	59	17	1732	1035	456	10	2.0	87	
								329	ulate

d on the 3D plane of the fault using the input of V-shale curves. The threshold

331 capillary pressures were calculated using two different SGR calibration techniques:

and deterministic. Both of these methods require an input of the maximum

- burial depth. The empirical method uses the burial depth to categorize faults for
- three different seal envelopes (< 3 km, 3 3.5 km, 3.5 5 km), while the
- 335 deterministic method directly incorporates the value. The deterministic method
- additionally requires an estimate of the depth at the time of faulting and a conversion
- 337 factor from mercury-air to gas-brine system, which is dependent on the interfacial
- tension between the wetting and non-wetting phases and the wettability of the
- 339 system. A minimum and maximum estimate of each of the parameters were
- 340 determined based on known reservoir conditions and a literature review, resulting in
- 341 two and eight possible scenarios for the empirical and deterministic methods,
- 342 respectively (Fig. 3). Both of these methods ascribe threshold capillary pressures to
- 343 every point of the 3D fault surface. These can then be compared to the known
- buoyancy pressure exerted by the gas column trapped in the reservoir.

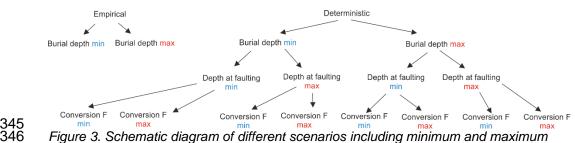


Figure 3. Schematic diagram of different scenarios including minimum and ma
 sestimates of parameters required by the empirical and deterministic methods.

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S

349 4.1.3 Input parameters

- 350 The input parameters used in the fault seal modelling are summarised in
- 351 Table 2, and the reasoning is explained below.

Field	Burial depth (m) (for deterministic)		Burial depth (m) (for empirical)		Depth at the time of faulting (m)		Conversion factor	
	min	max	min	max	min	max	min	max
Boggy Creek	1623	1783	<3000	-	450	1200	0.054	0.087
Katnook	2787	2987	<3000	3000- 3500	800	1200	0.111	0.133

352 Table 2. Summary of parameters used in fault seal modelling

353

354

355

4.1.3.1 Maximum burial depth

356 The Otway Basin has undergone two significant phases of uplift and 357 denudation, but the effects are less significant at the margins of the basin where the 358 two case studies are situated. A comprehensive basin-wide sonic transit time study 359 by (Tassone et al., 2014) suggests that Port Campbell is close to its maximum burial 360 depth, with a net exhumation range obtained from Boggy Creek-1 indicating 0 - 160 361 m net exhumation. The same is true for Penola Trough, where conservative 362 estimate of net exhumation is in the range of 0 - 200 m. This is confirmed by vitrinite 363 reflectance and apatite fission track data (Boult and Hibburt, 2002; Duddy, 1997). 364 The upper end of this range gives a maximum burial depth of 2987 m, which is very 365 close to the cut-off value of 3 km between different seal envelopes in Yielding et al. 366 (2010) method. We therefore consider two scenarios of < 3 km and 3 - 3.5 km maximum burial depth for the Penola Trough. 367

368

4.1.3.2 Depth at the time of faulting

369 4.1.3.2.1 Penola Trough

The main faulting event was contemporaneous with the Early Cretaceous rifting which coincided with the deposition of the regional seal formation. The sediments of the Crayfish Group commonly drape over major structural highs, indicating that faulting had ceased by the end of its deposition (Briguglio et al., 2015) and was inactive during the deposition of the overlying Eumeralla Formation (Boult et al., 2008), which is also evident from the seismic data. The depth of Ladbroke
Grove fault at the time of displacement is therefore constrained by the total
thickness of the Crayfish Group. The current thickness of the Crayfish Group in the
Katnook well is 800 m, which is also the thickest in the Penola Graben. Structural
cross-section balance and restoration indicates that 400 m of Crayfish sediments
were removed in the Penola Graben (Briguglio et al., 2015). Depth at the time of
faulting is therefore constrained to 800 - 1200 m.

382 4.1.3.2.2 Port Campbell

The seal formation, consisting of a succession of mudstones overlain by Skull Creek mudstone, varies in thickness across the faults, indicating synsedimentary faulting (Ziesch et al., 2015). The faulting ceased during the deposition of the unconformably overlain Wangerrip Group in Paleocene. Depth at the time of faulting is therefore represented by the thickness of this group, which ranges from 450 to 1200 m.

389 4.1.4 **Conversion factor**

390 The conversion factor from mercury-air to the chosen wetting and non-391 wetting phase requires an input of IFT and contact angle:

$$392 \qquad P_{wn} = P_{ma} \times \frac{IFT_{wn} \times cos\theta_{wn}}{IFT_{ma} \times cos\theta_{ma}}$$
(4)

393 where P is threshold capillary pressure, θ is the contact angle, w*n* and *ma* denote 394 wetting/non-wetting phase of choice and mercury/air, respectively.

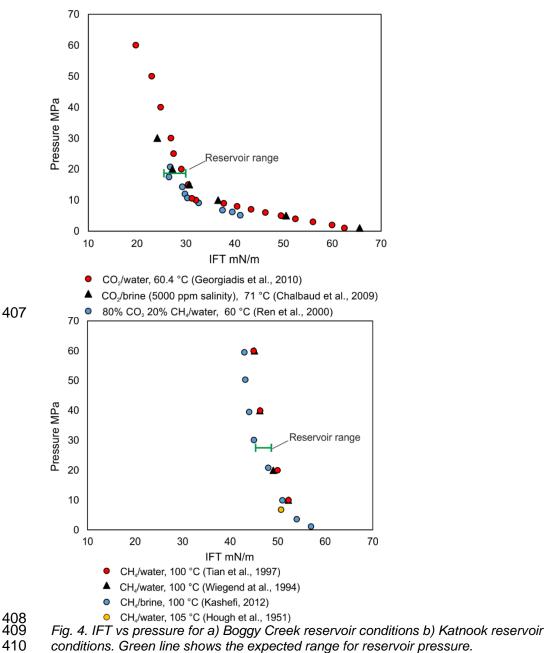
395 IFT has a strong dependency on pressure and temperature for both CO₂ 396 and methane, so assessment for local reservoir conditions is imperative. Figure 4 397 shows a compilation of results selected from laboratory studies under conditions 398 similar to those in Boggy Creek and Katnook reservoirs. Presented data include 399 CH₄-water, CO₂-water, CO₂-brine and CO₂-CH₄ mixtures in water (Chalbaud et al., 400 2009; Georgiadis et al., 2010; Hough et al., 1951; Kashefi, 2012; Ren et al., 2000; 401 Wiegand and Franck, 1994; Yi-Ling et al., 1997). The range constrained for the 402 Boggy Creek field is 26 - 32 mN/m (Fig. 4). Admixture of CH₄ to pure CO₂ generally 403 increases the IFT, but as shown in Figure 4a, the measurements in mixtures

404 containing < 20% methane are not significantly different from CO₂-water system

405 (Ren et al., 2000). The IFT range expected in Katnook methane field is 47-49 mN/m

406

(Fig. 4b).



410 411 412

Typical reservoir rocks are often considered to be water-wet in the presence

413 of hydrocarbons (e.g. Schowalter, 1974; Vavra et al., 1992), with some exceptions,

414 including grain coating with high polarity of crude oil components (Singh et al., 2016).

- 415 The Penola Trough traps show evidence for early charge of oil which was later
- displaced by gas (Higgs et al., 2015; Lovibond et al., 1995), therefore a range of 0-

30° contact angles is taken to reflect the potential effect of acid adsorption on grainsurfaces.

419 The wettability of CO₂-brine-mineral system has been investigated by a 420 growing number of studies (Bikkina, 2011; Farokhpoor et al., 2013; Jung and Wan, 421 2012), most commonly directly on single mineral surfaces, where minerals are 422 required to be ultraclean and smooth on an atomic level for reproducible results. The 423 results are highly variable (0 - 90°), but much of the variation is attributed to the 424 surface roughness and sample preparation practices (Iglauer et al., 2015). However, 425 the most consistent findings include a contact angle increase by up to 30° at CO₂ 426 transition from the gaseous to the supercritical phase (Jung and Wan, 2012; 427 Sutjiadi-Sia et al., 2008). In the absence of minerals known to be particularly 428 hydrophobic in the presence of CO₂ in the reservoir, the expected contact angle 429 range for Boggy Creek is taken to be 10 - 40°, as expected for common silicate and 430 carbonate reservoir minerals (Espinoza and Santamarina, 2010). 431 Given the defined range of IFT and contact angles for both reservoirs, 432 minimum and maximum conversion factors calculated for Boggy Creek Field (CO2-

433 dominated) and Katnook Field (methane-dominated) were 0.054 - 0.087 and 0.111 -

434 0.133, respectively.

437 **5 Results**

438 5.1 Juxtaposition

439 The Allan diagrams in Figure 5 show the juxtaposition of lithologies along the 440 strike of the fault planes for Katnook (a) and Boggy Creek (b) reservoirs. The 441 Katnook reservoir is primarily sealed by sand on shale juxtaposition by the Katnook 442 fault to the north, but the field extends to the hanging wall of the Ladbroke Grove 443 fault which is supporting the column to the south (Fig. 7.5a). The entire extent of the 444 reservoir is juxtaposed against reservoir on the other side of the fault. Similarly, the 445 Boggy Creek field is supported by sand on shale juxtaposition in the footwall of the 446 Boggy Creek fault to the south. The field extends to the hanging wall of the Buttress 447 fault (Fig. 5b), where the reservoir is self-juxtaposed for the entire extent of the gas 448 field. Calculated V-shale values for areas of reservoir self-juxtaposition range 449 between 20 and 50% on the Ladbroke Grove Fault and 10% to 80% on the Buttress 450 fault. SGR values above 20% are considered to be sealing (Yielding et al., 2010), so 451 in both cases the model indicates that the faults are acting as barriers to gas 452 migration.

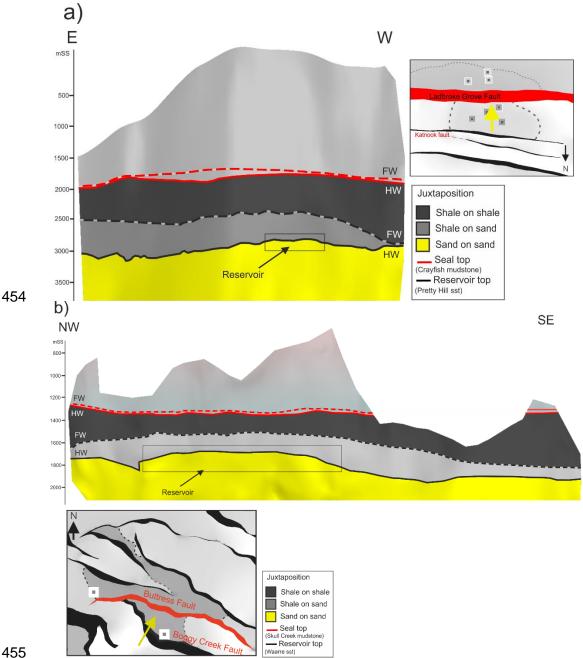


Figure 5. Allan diagrams showing juxtaposition along the strike-view of the faults, viewed 457 from the hanging wall side. Insets show the location of the faults (marked in red), the yellow 458 arrows show the direction of view. a) Ladbroke Grove fault, supporting the southern side of 459 the Katnook gas field (3x vertical exaggeration). b) Buttress fault, supporting the northern side of the Boggy Creek gas field (no vertical exaggeration). Black rectangles show the 460 461 extent of the gas-bearing reservoir. Horizon intersections on the fault plane are displayed as 462 dashed lines for the footwall side and solid lines for the hanging wall side.

465 5.2 Threshold capillary pressure

Across fault leakage through capillary seal breach commonly occurs near the top of the trap structure, where buoyancy pressure is the highest. The critical (and therefore most likely to leak) points occur where the lowest SGR values coincide with the highest buoyancy pressure on a given fault plane. The buoyancy pressure values identified at these points are 0.28 MPa for the Katnook field and 0.29 MPa for the Boggy Creek.

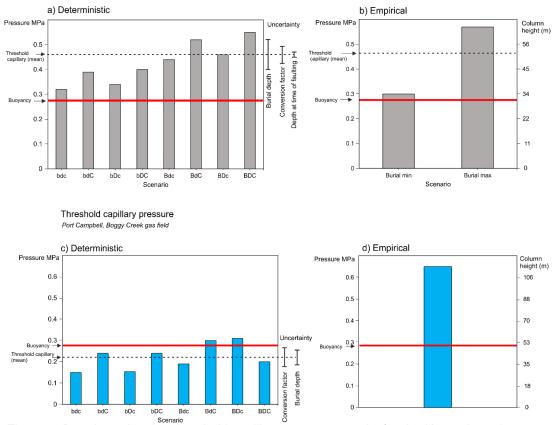
The calculated threshold capillary and buoyancy pressures can then be compared at the critical points, where the difference between them represents the amount of extra pressure (or extra gas column) the fault can retain before seal breach. Figure 6 shows the results of the deterministic (a, c) and empirical (b, d) calibrations for Katnook and Boggy Creek fields.

477 The results from both calibrations for the Katnook methane gas field indicate 478 that the current live gas column of 31 metres (equivalent to 0.28 MPa buoyancy 479 pressure) is stable but the fault is close to being critically pressured. The threshold 480 capillary pressures range from 0.32 to 0.55 MPa, equivalent to a total column of gas 481 between 35 to 57 m according to the deterministic calibration. Empirical calibration 482 suggests the fault seal will be breached at pressures between 0.3 and 0.57 MPa, 483 equivalent to a total gas column of 33 to 63 m. The results from both calibrations are 484 remarkably similar, with the average threshold capillary pressure of 0.42 and 0.43 485 MPa using the deterministic and empirical methods respectively.

486 The deterministic and empirical methods provide different results for the 487 Boggy Creek CO₂ field. The fault is currently supporting a 51 m column of gas, 488 equivalent to a buoyancy pressure of 0.29 MPa. This is close to the upper range 489 values predicted by the deterministic method. The threshold capillary pressure 490 ranges from 0.15 to 0.31 MPa (26 – 55 m of total column height). The predicted 491 average column height is 39 m, slightly under-predicting the sealing potential of the 492 fault. In contrast, the empirical calibration indicates a threshold pressure of 0.65 493 MPa and a maximum column height of 115 m, which is more than double the current 494 amount.

The empirical method requires only one parameter of the maximum burial depth. The deterministic method requires three parameters. In the case of the Katnook methane field, the uncertainty in maximum burial depth has the biggest impact on the results and the conversion factor is the second largest uncertainty (see y axis annotation on Fig. 6). In contrast, the uncertainty in the conversion factor has a greater impact on the Boggy Creek CO₂ field results than the maximum burial depth.

502 The structural spill point at the Katnook field is identified at 2891 m, which 503 effectively allows a maximum gas column height of 81 m. In Boggy Creek, the 504 structural spill point occurs at 1956 m, allowing a maximum column height of 272 m. 505 The maximum column heights identified from the structural perspective of the traps 506 are all higher than those modelled by fault seal analysis. This means that filling the 507 traps to the maximum fault-rock threshold pressures derived from all models would 508 not result in fill-to-spill and therefore both methods indicate that migration to the 509 adjacent fault trap occurred through the fault rather than through over-spilling.



510

Threshold capillary pressure Penola Trough, Katnook gas field

511 512 Figure 6. Bar chart showing threshold capillary pressure results for the Katnook methane 513 field (a, b) and the Boggy Creek CO₂ field (c, d) using deterministic (a, c) and empirical (b, d) 514 SGR calibration algorithms. Conversion to column height displayed on the secondary y axis 515 (same values applicable to both deterministic and empirical method graphs. Red line shows 516 current column height/buoyancy pressure. The Katnook gas column is predicted to be stable 517 by both methods with maximum threshold capillary pressure ranging from 0.32 to 0.55 MPa 518 (deterministic) and 0.3 to 0.57 MPa (empirical). The Boggy Creek field is predicted to be 519 within the upper end of the critical pressure zone by the deterministic method (0.15-0.31 520 MPa) and stable by the empirical method. Labels in deterministic scenarios: B- maximum 521 burial depth, D – depth at the time of faulting, C – conversion factor. Upper and lower case 522 letter indicate maximum and minimum values respectively.

524 6 Discussion

525 6.1 Addressing the uncertainty in fault seal modelling

526 The deterministic and empirical methods present a key difference in their 527 definition of the threshold capillary pressure. The deterministic method defines a best fit line through the data points of measured capillary entry pressures during 528 529 injection experiments to fault rock samples. Therefore, by definition, the method 530 predicts the average threshold pressure for the modelled conditions. In contrast, the 531 fault seal envelopes defining the threshold capillary pressure in the empirical 532 method represent the upper limit of data for buoyancy pressures retained by fault 533 rocks with a given SGR. The threshold pressure returned by the empirical equation 534 is therefore a maximum estimate. In other words, even though the same term of 535 threshold capillary pressure is used by the two methods, the derived value 536 represents somewhat different concepts and presents a different level of uncertainty.

537 Some uncertainties are inherent to the modelling method and cannot be 538 easily accounted for. The deterministic method is based on threshold capillary 539 pressure measurements of micro-fault samples on the scale of millimetres to 540 centimetres (Sperrevik et al., 2002). The measured clay content of the fault 541 structures is assumed to be represented by SGR when upscaled to use in a 542 predictive way. The method is therefore applied on the assumption that kilometre 543 scale faults behave in the same way as micro structures. In reality this is not strictly 544 the case, with seismic-scale fault zones comprising clay smears, cataclastic zones 545 and multiple planes of deformation (Bense et al., 2016; Faulkner et al., 2010; Fisher 546 and Knipe, 1998; Pei et al., 2015; Shipton and Cowie, 2001), which all add to the 547 total sealing capacity of the fault zone. Detailed fault zone analyses show that the 548 permeability over individual fault zone components can vary considerably (e.g. over 549 3 orders of magnitude) (Shipton et al., 2002) and therefore upscaling one of those 550 components to be representative of the entire fault zone involves a significant 551 simplification.

552 The advantage of the empirical method in this respect is that SGR is 553 assumed to be a proxy for the fault sealing properties, which include shale content

554 but also various heterogeneous components of the fault zone. SGR calculated on 555 the 3D surface of the fault planes is the direct input in the calibration as well as in 556 the predictive workflow, which eliminates the uncertainty associated with equating 557 SGR to specific rock properties such as the true volume of shale. The compilation 558 dataset includes data from 7 different basins, covering a wider range of diagenetic 559 conditions relative to the deterministic method which is based on samples from the 560 North Sea (Yielding, 2002).

561 Some of the uncertainties associated with the local geological conditions and 562 fluid properties are parameterised in the deterministic method and therefore can be 563 accounted for. The error bars in Figure 6 a) and c) show the relative uncertainties 564 associated with the different model input parameters. For the two case studies 565 presented here, fluid properties (governing the conversion factor) present a higher uncertainty for CO₂ rather than methane. This is primarily due to the larger IFT 566 567 range selected for CO_2 , but does not suggest that the interfacial tension of CO_2 is 568 less characterised than that of methane. The larger range is due to a relatively 569 higher number of currently available studies, including measurements using different 570 salinity, salt types and gas mixtures, while methane laboratory studies are largely 571 constrained to pure methane and deionized water. In cases where fluid properties 572 are well defined, maximum burial depth is the most significant source of uncertainty, 573 while depth at the time of faulting is the least significant input parameter.

6.2 Uncertainty related to fluid properties

An important difference between the two methods is the approach to 575 576 accounting for the fluid properties. The interfacial tension and wettability are 577 parameterised in the deterministic method, making it more versatile, arguably 578 adaptive to CO₂-brine system and more precise in cases where fluid properties are 579 well characterised. The empirical method does not explicitly address the fluid 580 properties, but operates under the assumption that the range of IFT and contact 581 angle configurations in hydrocarbons is small, and that the possible variability of 582 fluid properties is represented in the global dataset compilation. The two important 583 issues with the empirical approach are:

a) the uncertainty related to fluid properties is undefined when applied tohydrocarbons.

b) the application to CO_2 can only be considered valid in cases where CO_2

587 exhibits properties within the range of those observed in hydrocarbons.

588 These are explained in detail below.

6.3 a) Uncertainty related to fluid properties of hydrocarbons in the empirical model

591 To further assess the empirical method application to CO_2 , the uncertainty 592 related to the fluid properties of hydrocarbons has to be defined. The percentage 593 error of the capillary threshold pressure (δP_c) from the uncertainty in fluid properties

594 (as standard deviation) can therefore be expressed as, using Equation 1:

595
$$\delta P_c = \frac{\sigma(P_c)}{\partial(P_c)} \times 100\% = \frac{\sigma(2IFT \times cos\theta)}{\partial(2IFT \times cos\theta)} \times 100\%$$
(5)

596 The empirical method uses a data compilation including both oil and 597 methane in reservoirs > 1.5 km depth (Yielding, 2002), and can be assumed to 598 reflect the general IFT and contact angle variability of all hydrocarbons at that depth. 599 The percentage error can therefore be calculated using a random sampling 600 modelling approach with inputs of the probability distribution of IFT and contact 601 angle values in hydrocarbons-brine system. Interfacial tension and contact angle are 602 assumed to be independent variables; even though some co-variation may exist, 603 currently it is not well understood and there are far more factors affecting the contact 604 angle not directly related to the fluid type.

605 6.3.1 Defining IFT and wettability range for hydrocarbons

606 The IFT between hydrocarbons and water (or brine) is primarily controlled by 607 the chemical composition of the hydrocarbons, the density contrast between the two 608 phases and temperature (Flock et al., 1986; Hassan et al., 1953; Rajayi and 609 Kantzas, 2011). Pressure mainly affects gas solubility in oil and therefore has a 610 bigger effect on oils with high dissolved gas content (Ghorbani and Mohammadi, 611 2017). Generally, the IFT in hydrocarbons is not well characterised and usually an 612 average IFT of 30-35 mN/m is used for capillary seal modelling purposes (Berg, 613 1975; Robert M. Sneider and Neasham, 1997). Considerable effort has been made

614 to characterise IFT of individual hydrocarbon compounds and derive predictive

615 equations to determine the IFT based on the input of reservoir temperature

616 (Kalantari Meybodi et al., 2016), density difference (Danesh, 1998; Sutton, 2006)

and critical fluid temperature (Najafi-Marghmaleki et al., 2016). However, these

618 methods are developed for data compilations of pure aromatics and alkanes, and do

not reflect the fluid properties of crude oil at reservoir conditions, which include high

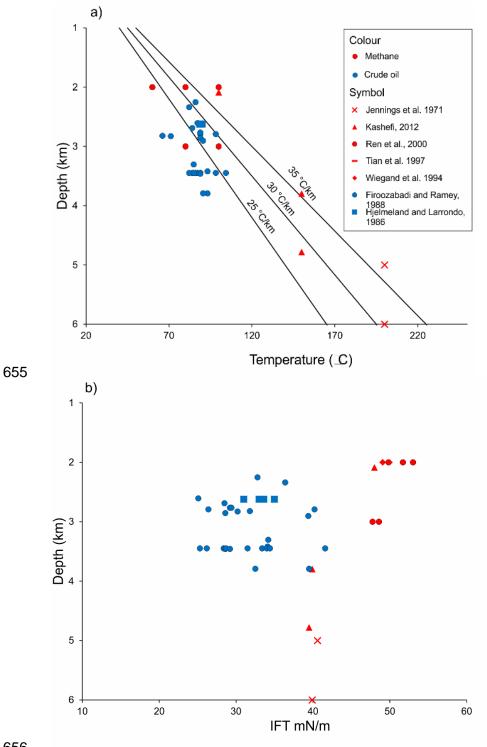
620 percentage of other compounds such as napthenes and asphaltics (Buckley et al.,

621 1997).

622 There have been relatively few studies presenting IFT measurements in 623 crude oil-water systems, but these can be considered the most reservoir-624 representative. Figure 8 shows a compilation of laboratory measurements within the 625 envelope of pressures and temperatures valid for geothermal gradients between 25 626 and 35 °C/km and hydrostatic pressure gradient of 10 MPa/km. The compilation 627 includes samples of crude oil above bubble point representing non-degassed oils, 628 below-bubble point oils and methane. The IFT values of crude oil range 26-42 mN/m 629 and are more strongly controlled by chemical differences rather than depth. IFT of 630 methane decreases with depth and ranges from 40 to 53 mN/m. Based on this 631 example dataset, it is assumed that the IFT values of hydrocarbons used in the 632 empirical calibration method are expected to be within a uniform probability 633 distribution with a mean value of 39 ± 8 mN/m (Fig. 9a).

634 In the context of capillary seal modelling, reservoir formations are generally 635 considered to be water-wet in the presence of hydrocarbons (contact angle = 0°) 636 (e.g. Schowalter, 1974; Vavra et al., 1992). This is not strictly true, with mixed-wet 637 and oil-wet states often observed in hydrocarbon reservoirs (Treiber and Owens, 638 1972), often due to mineral surface coating with high polarity crude oil components 639 such as asphaltenes which have high affinity to the reservoir minerals (Alipour 640 Tabrizy et al., 2011; Singh et al., 2016). The degree of oil-wetting is expected to be 641 higher in reservoirs containing high maturity oil and in the presence of carbonate 642 cements, smectite, chlorite, kaolinite and iron-oxides (Barclay and Worden, 2009; 643 Worden and Morad, 2000). Because the contact angle directly affects the calculated 644 column heights and associated threshold capillary pressures, the practice of 645 assuming 0° contact angle in hydrocarbon reservoirs always provides a maximum 646 rather than conservative estimate. In the absence of strong statistical data, we 647 assume that reservoir rocks are more commonly water-wet than oil-wet in the

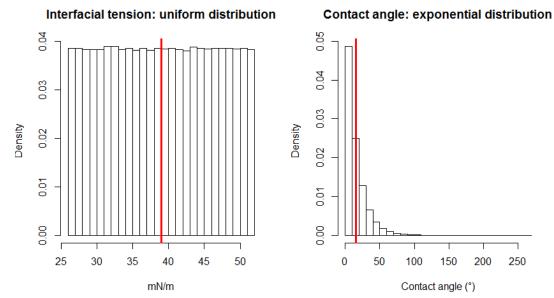
- 648 presence of hydrocarbons. This spread of data is best described by an exponential
- 649 probability distribution (β = 15), with a mean value of $15 \pm 15^{\circ}$ (Fig 9b) The lowest
- values in the range are the most probable. Based on Equation 3, retention of a gas
- 651 column is only possible when the contact angle is $\leq 90^{\circ}$ (cos $\theta > 0$). Because the
- 652 data set by definition only includes reservoirs with observed columns, contact angles
- 653 must range between 0 and 90°.





656 657 658 Figure 8. IFT of crude oil and methane data compilation from the literature, filtered to 659 conditions applicable to geological pressure and temperature conditions (25 - 35 °C/km 660 geothermal gradient). a) shows the distribution depth vs temperature conditions, b) shows 661 the IFT values of the same data points. Crude oil IFT values range between 26 - 42 mN/m

and are uniformly distributed. Methane values range 40 - 53 mN/m and decrease with depth.
Combined together, this data represents a uniform distribution.



664 665 Figure 9. Probability distribution of IFT (a) and contact angle (b) in hydrocarbons at reservoir 666 conditions below 2 km depth, defined based on a literature review of laboratory studies 667 (discussed in text). Red vertical line shows mean. IFT is expected to be uniformly distributed 668 with a mean value of 39 ± 8 mN/m. Exponential distribution (β =15) best describes the 669 expected contact angle. 670

- Based on the probability distributions of IFT and contact angle determined above, the percentage error of threshold capillary pressure (δP_c) determined from
- 673 Equation 5 using Monte Carlo random sampling analysis (n = 10⁶) is 24%. Figure 10
- shows the seal failure envelopes of the empirical model (Yielding et al., 2010) with
- the calculated error added. The seal envelopes define the upper boundary of all
- 676 buoyancy pressures observed to be sealed by fault rocks and therefore statistically
- 677 represent the higher values within the data distribution or maximum threshold
- 678 capillary pressure. We can therefore use the calculated uncertainty to estimate the
- average threshold capillary pressure $(P_c \sigma)$ and minimum threshold capillary
- 680 pressure $(P_c 2\sigma)$. The uncertainty increases with increasing P_c .

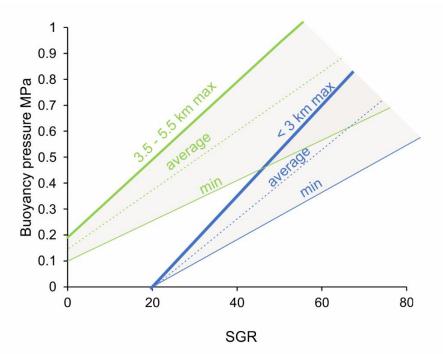


Figure 10. SGR vs Buoyancy pressure with < 3 km and 3.5 - 5.5 km threshold capillary
pressure envelopes from Yielding et al. (2010). The thick solid line shows the original
maximum threshold capillary pressure. Dashed lines show calculated average and minimum
pressures for given burial depth brackets.

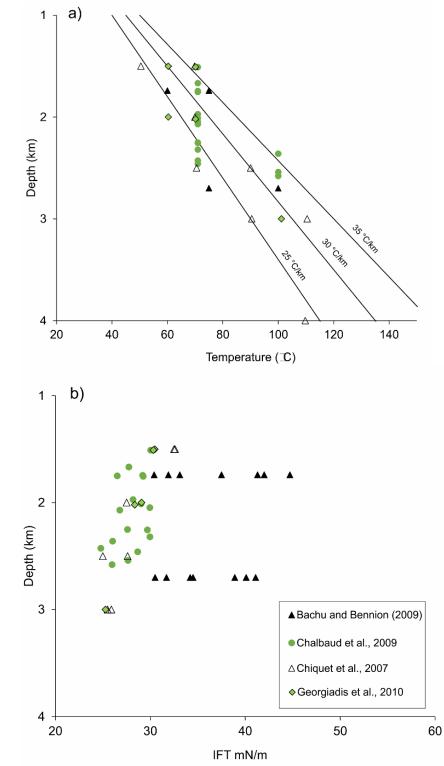
687 6.3.1.1 Implications for use in hydrocarbons

688 The calculated uncertainty envelopes do not change the interpretation of the 689 empirical calibration method, but rather provide additional constraints that can be 690 applied in variety of contexts. In cases where capillary pressure modelling is used to 691 assess the economic viability of the reservoir, the uncertainty can be a useful input 692 into the risking process. The average threshold capillary pressure value is better 693 used in the calculation of likely hydrocarbon column heights, bearing in mind that the 694 true column height can be controlled by many factors independent to fault seal such 695 as structural spill points and charge. In cases where sufficient geological evidence 696 exists to indicate that the trap has been filled, the calculated uncertainty envelope 697 provides means to determine the minimum expected column. The average threshold 698 capillary pressure value using the empirical method is also more comparable to the 699 average results of the deterministic method (rather than using the current empirical 700 max value) when the two are used in conjunction.

6.4 b) Empirical method applied to the fluid properties of

702 CO₂

703 In the last decade significant effort has gone into characterising IFT of CO₂ 704 at a range of conditions, with existing data covering CO₂/water (Chiquet et al., 705 2007a; Georgiadis et al., 2010) and CO_2 /brine with variable salinity and salt types 706 (Bachu and Bennion, 2009; Chalbaud et al., 2009). IFT has been characterised for 707 mixtures of CO_2 and methane in water (Ren et al., 2000) and brine (Liu et al., 2016). 708 Increasing brine salinity has been shown to increase the IFT in CO₂/brine system 709 with significant deviations in saline and hypersaline conditions (Bachu and Bennion, 710 2009; Chalbaud et al., 2009; Liu et al., 2016). Figure 11 shows results from 711 published laboratory studies filtered to those representative of pressure and 712 temperature conditions in the subsurface (geothermal gradients 25 – 35 °C/km, 713 hydrostatic pressure gradient 10 MPa/km). The data includes pressures above 15 714 MPa (~1.5 km depth), which is in line with depths recommended for safe geological 715 CO₂ sequestration (> 1.2 km) (Miocic et al., 2016). It is apparent that in the 716 supercritical fluid state, depth does not significantly influence the IFT. The most 717 important controlling factor is brine salinity which increases the IFT due to increasing 718 density contrast between CO₂ and the brine. The maximum IFT values of 44.7 and 719 41.1 mN/m at 1.7 km and 2.7 km depth respectively from the study of Bachu and 720 Bennion (2009) are measured in brines of 334 g/L salinity, which is close to the 721 maximum possible salt saturation in water. In comparison, the salinity of UK oil and 722 gas fields ranges from 30 to 227 g/L with an average value of 130 g/L (Gluyas and 723 Hichens, 2003). The IFT range presented here covers the minimum (CO₂-pure 724 water) to maximum (CO₂-hypersaline brine) geologically possible conditions relevant 725 to CO_2 sequestration context (> 1.5 km depth), and also falls within the range 726 observed in liquid hydrocarbons. The IFT values range between 26 to 45 mN/m, 727 which is remarkably similar to IFT range in crude oil (26 – 42 mN/m, Fig. 8).



728



Figure 11. IFT of CO₂ in water and brine of different salinities, filtered to only display pressure and temperature conditions applicable to geological setting (25-35 °C/km geothermal gradient). a) shows the distribution depth vs temperature conditions, b) shows the IFT values of the same data points. IFT ranges 26-45 mN/m. Datapoints from Bachu and Bennion (2009) show the effects of increasing salinity, with a maximum of 334 g/L resulting in the highest IFT values.

737 The wettability in CO₂-brine system is a complex issue and cannot be easily 738 defined as a bracket range for all reservoir conditions. The conditions of many 739 experimental set ups are very different to reservoir conditions, as discussed in 740 section 4.1.4, therefore the upscaling of single mineral experimental results to 741 reservoir is problematic Irrespective of this variation, the most significant observation 742 emerging from CO₂-brine lab studies is the change in wettability caused by pressure. 743 This is observed when CO₂ changes from gaseous to supercritical fluid phase at 744 around 8 MPa. It is presently not understood if the change in wettability is related to 745 the process of phase change or to the physical properties of supercritical CO₂.

In summary, the IFT values for CO₂ are similar to those of oil, while methane
IFT values are higher on average. The contact angles in CO₂-brine system present
a higher level of uncertainty and are hard to evaluate as a generic range. IFT and
contact angles can however be defined with higher confidence for specific reservoir
conditions, as exemplified by this study.

751 6.4.1 Conversion factor from hydrocarbons to CO₂

This work has defined an average value (μ) of the probability distributions of IFT (39 mN/m) and CA (15°) for hydrocarbons under pressure and temperature conditions included in the calibration dataset by Yielding et al. (2010). This means that the calculated threshold capillary pressure of hydrocarbons can be converted to CO₂-brine system for chosen IFT and CA values of CO₂:

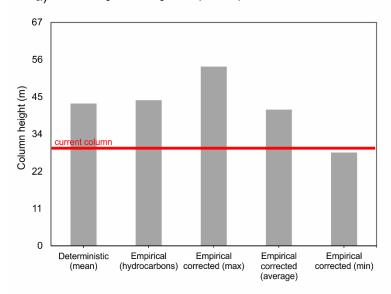
757
$$P_c(CO_2) = P_c \times \frac{IFT_{CO2} \times cos\theta_{CO2}}{\mu IFT_h \times \mu cos\theta_h}$$
(6)

This can also be applicable to hydrocarbons in instances where IFT and CA are well defined and significantly different to the average values.

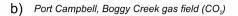
Figure 12 shows calculated column heights calculated using the standard empirical and deterministic methods, compared to the empirical model after conversion to CO₂ using Equation 6 (maximum value) and calculated average and minimum values. For the Katnook methane system, the correction factor increases the column heights for methane due to higher IFT, but the overall change is not significantly different from the original empirical model. The current column is predicted to be stable regardless of the correction. 767 The maximum column height for the Boggy Creek CO₂ field is reduced by 768 the correction, with the average empirical value slightly higher than the column 769 height value known to be held by the fault. This prediction is in closer agreement to 770 the deterministic model, and is more likely to be correct based on the geochemistry 771 of the fields, indicating higher mantle CO₂ contents at Boggy Creek than in the 772 adjacent Buttress field and suggesting initial charge to Boggy Creek lead to 773 subsequent migration into Buttress. The current column in Boggy Creek is not near 774 the structural spill point, suggesting the CO₂ transfer between the fields occurred 775 through the fault rock, and the current column is therefore expected to be near the 776 threshold value.

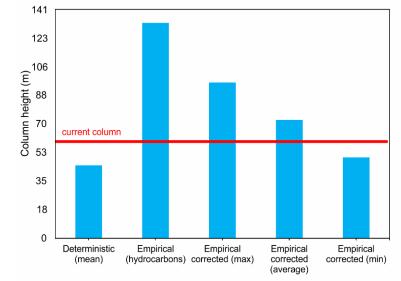
Gas column heights (m)

a) Penola Trough, Katnook gas field (methane)









778 779

79 Figure 12. Gas column heights a) Penola Trough, Katnook field b) Port Campbell, Boggy

780 Creek field. Current live columns marked in red. Models shown: deterministic (Sperrevik et al., 2002), empirical (Yielding et al., 2010), empirical corrected max, average and min values

782 (this work).

784 **7** Conclusions

Two gas fields sealed by fault rocks were examined to compare the standard fault seal analysis techniques applied to methane-brine and CO_2 -brine systems. In both cases, the column heights supported by the fault rocks were known, and geochemical gas analysis provided evidence for across-fault connectivity. This allowed us to assess and compare the strengths and weaknesses of two fault seal calibration methods (Sperrevik et al., 2002; Yielding et al., 2010).

The deterministic method predicted critical buoyancy pressure in Katnook (methane) and Boggy Creek (CO₂) fields. The empirical method predicted critical buoyancy pressure in Katnook field and well below threshold pressure in the Boggy Creek field. However, after accounting for uncertainty and applying the newly proposed correction for CO₂, the method also predicted criticality. Thus, the geochemistry and fault seal analysis results corroborate each other.

797 CO₂ fluid properties and their differences from hydrocarbons have been 798 previously identified as the biggest uncertainty associated with fault seal application 799 to CO₂ systems. However, an extensive literature review showed that a similar 800 spread in IFT values exists within the hydrocarbons, due to the wide range of 801 possible chemical compositions of crude oil. This means that IFT in CO₂-brine 802 system is easier to identify for particular pressure and temperature conditions than 803 in liquid hydrocarbons. Wettability of hydrocarbons is not very well characterised 804 either, and the recent academic focus to CO₂ sequestration applications means that 805 currently far more laboratory experimental data exists for CO₂-brine systems. 806 Perhaps surprisingly, the main challenge in adapting fault seal modelling techniques 807 from hydrocarbons to CO₂ is the uncertainty associated to the hydrocarbon 808 properties.

The two fault seal prediction methods discussed here come with different inherent uncertainties and are best used in conjunction, bearing in mind the differences in the approach. The deterministic method (Sperrevik et al., 2002) can be applied to different fluids via the input of IFT and CA. This work has presented a similar conversion factor system applied to the empirical method (Bretan et al., 2003; Yielding et al., 2010). To do this, an average range of IFT and CA in hydrocarbons 815 under reservoir conditions was determined from literature review. The uncertainty 816 related to the spread in fluid properties was calculated to be 24% of the calculated 817 threshold capillary pressure value. This finding does not change the application of 818 the empirical method, which by definition provides a maximum estimate for capillary 819 threshold pressures. However, it allows to constrain an average and minimum 820 capillary pressure values, which can be used to ascertain 'most likely' and minimum 821 column heights in hydrocarbon exploration. The newly defined average capillary 822 threshold pressure value also allows for better comparison with the deterministic 823 method, which by definition models average rather than maximum pressures.

824 The definition of average IFT and CA of the dataset in the empirical method 825 also allows the conversion of the threshold capillary pressures to other fluid systems, 826 which is desirable for the application to CO_2 sequestration. In application to CO_2 827 storage, where a full column is fully or partially sealed by a fault, the buoyancy 828 pressure must not exceed the minimum threshold capillary pressure value. However, 829 the minimum values discussed here do not equate to safe or recommended 830 buoyancy pressures for CCS contexts. Future studies should define the 831 recommended limit in relation to the minimum threshold capillary pressure values 832 defined here, based on risk analysis and regulatory guidelines.

833

834 8 Acknowledgments

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843 9 References

844 845 846 847	Alipour Tabrizy, V., Denoyel, R., Hamouda, A.A., 2011. Characterization of wettability alteration of calcite, quartz and kaolinite: Surface energy analysis. Colloids Surfaces A Physicochem. Eng. Asp. 384, 98–108. https://doi.org/10.1016/j.colsurfa.2011.03.021
848 849	Allan, U.S., 1989. Model for hydrocarbon migration and entrapment within faulted structures. Am. Assoc. Pet. Geol. Bull. 73, 803–811.
850 851 852	Andrew, M., Bijeljic, B., Blunt, M.J., 2014. Pore-scale contact angle measurements at reservoir conditions using X-ray microtomography. Adv. Water Resour. 68, 24–31. https://doi.org/10.1016/J.ADVWATRES.2014.02.014
853 854	Asquith, G.B., Krygowski, D., Gibson, C.R., 2004. Basic well log analysis. American Association of Petroleum Geologists Tulsa.
855 856 857 858	Bachu, S., Bennion, D.B., 2009. Interfacial tension between CO2, freshwater, and brine in the range of pressure from (2 to 27) MPa, temperature from (20 to 125) °C, and water salinity from (0 to 334 000) mg L-1. J. Chem. Eng. Data 54, 765–775. https://doi.org/10.1021/je800529x
859 860 861	Barclay, S.A., Worden, R.H., 2009. Effects of reservoir wettability on quartz cementation in oil fields. Quartz Cem. sandstones (Eds RH Worden S. Morad). Spec. Pubilication 29, 103–117.
862 863 864	Bense, V.F., Shipton, Z.K., Kremer, Y., Kampman, N., 2016. Fault zone hydrogeology: introduction to the special issue. Geofluids 16, 655–657. https://doi.org/10.1111/gfl.12205
865	Berg, R.R., 1975. Capillary Pressures in Stratigraphic Traps'.
866 867 868	Bikkina, P.K., 2011. Contact angle measurements of CO2–water– quartz/calcite systems in the perspective of carbon sequestration. Int. J. Greenh. Gas Control 5, 1259–1271. https://doi.org/10.1016/J.IJGGC.2011.07.001
869 870	Boreham, C.J., Hope, J.M., Jackson, P., Davenport, R., Earl, K.L., Edwards, D.S., Logan, G.A., Krassay, A.A., 2004. Gas – oil – source correlations in the Otway

Basin, southern Australia. Petroleum Exploration Society of Australia (PESA), pp.19–22.

Boult, P., Lyon, P., Camac, B., Hunt, S., Zwingmann, H., 2008. Unravelling
the complex structural history of the Penola Trough – revealing the St George Fault.
PESA East. Australas. Basins Symp. III 14–17.

Boult, P.J., Hibburt, J.E., 2002. The petroleum geology of South Australia.
Vol. 1: Otway Basin. 2nd edn. South Australia. Department of Primary Industries
and Resources. Petroleum Geology of South Australia Series, Vol. 1.

Boult, P.J., Johns, D.R., Lang, S.C., 2004. Subsurface plumbing of the
Crayfish Group in the Penola Trough: Otway Basin, in: Eastern Australasian Basins
Symposium II. Petroleum Exploration Society of Australia (PESA), pp. 483–498.

Bretan, P., Yielding, G., Jones, H., 2003. Using calibrated shale gouge ratio
to estimate hydrocarbon column heights. Am. Assoc. Pet. Geol. Bull. 87, 397–413.
https://doi.org/10.1306/08010201128

Bretan, P., Yielding, G., Mathiassen, O.M., Thorsnes, T., 2011. Fault-seal
analysis for CO2 storage: an example from the Troll area, Norwegian Continental
Shelf. Pet. Geosci. 17, 181–192. https://doi.org/10.1144/1354-079310-025

888 Briguglio, D., Hall, M., Keetley, J., 2015. Structural evolution of the Early 889 Cretaceous depocentres, Otway Basin, Victoria. Aust. J. Earth Sci. 1–17.

890 https://doi.org/10.1080/08120099.2015.1084048

891 Buckley, J.S., Liu, Y., Xie, X., Morrow, N.R., 1997. Asphaltenes and crude oil 892 wetting-the effect of oil composition. SPE J. 2, 107–119.

Chalbaud, C., Robin, M., Lombard, J.-M., Martin, F., Egermann, P., Bertin,

H., 2009. Interfacial tension measurements and wettability evaluation for geological

895 CO2 storage. Adv. Water Resour. 32, 98–109.

- 896 https://doi.org/10.1016/J.ADVWATRES.2008.10.012
- 897 Chiquet, P., Daridon, J.-L., Broseta, D., Thibeau, S., 2007a. CO2/water 898 interfacial tensions under pressure and temperature conditions of CO2 geological

- storage. Energy Convers. Manag. 48, 736–744.
- 900 https://doi.org/10.1016/j.enconman.2006.09.011
- 901 Chiquet, P., Daridon, J.L., Broseta, D., Thibeau, S., 2007b. CO2/water
- 902 interfacial tensions under pressure and temperature conditions of CO2 geological
- storage. Energy Convers. Manag. 48, 736–744.
- 904 https://doi.org/10.1016/j.enconman.2006.09.011
- 905Chivas, A.R., Barnes, I., Evans, W.C., Lupton, J.E., Stone, J.O., 1987. Liquid906carbon dioxide of magmatic origin and its role in volcanic eruptions. Nature 326,
- 907 587–589. https://doi.org/10.1038/326587a0
- Cockshell, C.D., O'Brien, G.W., McGee, A., Lovibond, R., Perincek, D.,
 Higgins, R., 1995. Western Otway Crayfish Group troughs. APPEA J. 35, 385–404.
- 910 Dance, T., 2013. Assessment and geological characterisation of the
- 911 CO2CRC Otway Project CO 2 storage demonstration site: From prefeasibility to
- 912 injection. Mar. Pet. Geol. 46, 251–269.
- 913 https://doi.org/10.1016/j.marpetgeo.2013.06.008
- Danesh, A., 1998. PVT and phase behaviour of petroleum reservoir fluids.Elsevier.
- 916 Daniel, R.F., Kaldi, J.G., 2009. Evaluating Seal Capacity of Cap Rocks and
- 917 Intraformational Barriers for CO 2 Containment 335–345.

918 https://doi.org/10.1306/13171247St59227

- Duddy, I.R., 1997. Focussing exploration in the Otway Basin: understanding
 timing of source rock maturation. APPEA J. 37, 178–191.
- 921 Espinoza, D.N., Santamarina, J.C., 2010. Water-CO2 -mineral systems:
 922 Interfacial tension, contact angle, and diffusion-Implications to CO2 geological
 923 storage. Water Resour. Res. 46. https://doi.org/10.1029/2009WR008634
- 924 Jennings, H.Y., Newman, G.H., 1971. The effect of temperature and
- pressure on the interfacial tension of water against methane-normal decane
 mixtures. Soc. Pet. Eng. J. 11, 171–175.

- 927 Farokhpoor, R., Bjørkvik, B.J.A., Lindeberg, E., Torsæter, O., 2013. CO2 928 Wettability Behavior During CO2 Sequestration in Saline Aguifer -An Experimental 929 Study on Minerals Representing Sandstone and Carbonate. Energy Procedia 37, 930 5339-5351. https://doi.org/10.1016/J.EGYPRO.2013.06.452 931 Faulkner, D.R., Jackson, C.A.L., Lunn, R.J., Schlische, R.W., Shipton, Z.K., 932 Wibberley, C.A.J., Withjack, M.O., 2010. A review of recent developments 933 concerning the structure, mechanics and fluid flow properties of fault zones. J. Struct. 934 Geol. 32, 1557-1575. 935 Firoozabadi, A., Ramey, H.J., Ramey Jr, H.J., 1988. Surface tension of 936 water-hydrocarbon systems at reservoir conditions. J. Can. Pet. Technol. 27. 937 Fisher, Q.J., Knipe, R.J., 1998. Fault sealing processes in siliciclastic 938 sediments. Geol. Soc. London, Spec. Publ. 147, 117-134. https://doi.org/10.1144/GSL.SP.1998.147.01.08 939 940 Flock, D.L., Le, T.H., Gibeau, J.P., 1986. The effect of temperature on the 941 interfacial tension of heavy crude oils using the pendent drop apparatus. J. Can. Pet. 942 Technol. 3. 943 Georgiadis, A., Maitland, G., Trusler, J.P.M., Bismarck, A., 2010. Interfacial
- 944 tension measurements of the (H2O + CO2) system at elevated pressures and

945 temperatures. J. Chem. Eng. Data 55, 4168–4175.

- 946 https://doi.org/10.1021/je100198g
- 947 Ghorbani, M., Mohammadi, A.H., 2017. Effects of temperature, pressure and
- 948 fluid composition on hydrocarbon gas oil interfacial tension (IFT): An experimental
- study using ADSA image analysis of pendant drop test method. J. Mol. Liq. 227,

950 318–323. https://doi.org/10.1016/J.MOLLIQ.2016.11.110

- Gibson, R.G., 1998. Physical character and fluid-flow properties of
 sandstone-derived fault zones. Geol. Soc. London, Spec. Publ. 127, 83–97.
- 953 Gluyas, J.G., Hichens, H.M., 2003. United Kingdom oil and gas fields: 954 commemorative millennium volume.

- Guariguata-Rojas, G.J., Underhill, J.R., 2017. Heriot-Watt University
 Implications of Early Cenozoic uplift and fault reactivation for carbon storage in the
 Moray Firth Basin Implications of Early Cenozoic uplift and fault reactivation for
 carbon storage in the Moray Firth Basin. https://doi.org/10.1190/int-2017-0009.1
- Hassan, M.E., Nielsen, R.F., Calhoun, J.C., 1953. Effect of Pressure and
 Temperature on Oil-Water Interfacial Tensions for a Series of Hydrocarbons. J. Pet.
 Technol. 5, 299–306. https://doi.org/10.2118/298-G
- Higgs, K.E., Haese, R.R., Golding, S.D., Schacht, U., Watson, M.N., 2015.
 The Pretty Hill Formation as a natural analogue for CO2 storage: An investigation of
 mineralogical and isotopic changes associated with sandstones exposed to low,
 intermediate and high CO2 concentrations over geological time. Chem. Geol. 399,
 36–64. https://doi.org/10.1016/j.chemgeo.2014.10.019
- 967 Hjelmeland, O.S., Larrondo, L.E., 1986. Experimental Investigation of the
 968 Effects of Temperature, Pressure, and Crude Oil Composition on Interfacial
 969 Properties. SPE Reserv. Eng. 1, 321–328. https://doi.org/10.2118/12124-PA
- Hough, E.W., Rzasa, M.J., Wood, B.B., Oil, S., Co, G., 1951. Interfacial
 Tensions at Reservoir Pressures and Temperatures ; Apparatus and the WaterMethane System. J. Pet. Trans. AIME 192, 57–60. https://doi.org/10.2118/951057-G
- 973 Iglauer, S., 2018. Optimum storage depths for structural CO2 trapping. Int. J.
 974 Greenh. Gas Control 77, 82–87. https://doi.org/10.1016/J.IJGGC.2018.07.009
- Iglauer, S., Pentland, C.H., Busch, A., 2015. CO2 wettability of seal and
 reservoir rocks and the implications for carbon geo-sequestration. Water Resour.
 Res. 51, 729–774. https://doi.org/10.1002/2014WR015553
- Jung, J.-W., Wan, J., 2012. Supercritical CO 2 and Ionic Strength Effects on
 Wettability of Silica Surfaces: Equilibrium Contact Angle Measurements. Energy &
 Fuels 26, 6053–6059. https://doi.org/10.1021/ef300913t
- Kalantari Meybodi, M., Daryasafar, A., Karimi, M., 2016. Determination of
 hydrocarbon-water interfacial tension using a new empirical correlation. Fluid Phase
 Equilib. 415, 42–50. https://doi.org/10.1016/J.FLUID.2016.01.037

Karolytė, R., 2018. The migration and retention of CO2 and methane in the
Otway Basin and south-east Australia: an integrated geochemical and structural
analysis. University of Edinburgh.

Karolytė, R., Johnson, G., Györe, D., Serno, S., Flude, S., Stuart, F.M.,
Chivas, A.R., Boyce, A., Gilfillan, S.M.V., 2019. Tracing the migration of mantle CO2
in gas fields and mineral water springs in south-east Australia using noble gas and
stable isotopes. Geochim. Cosmochim. Acta 259, 109–128.

Kashefi, K., 2012. Measurement and modelling of interfacial tension andviscosity of reservoir fluids. Thesis. Heriot-Watt University.

Knipe, R.J., 1997. Juxtaposition and seal diagrams to help analyze fault
seals in hydrocarbon reservoirs. Am. Assoc. Pet. Geol. Bull. 81, 187–195.

995 Lehner, F.K., Pilaar, W.F., 1997. The emplacement of clay smears in

996 synsedimentary normal faults: inferences from field observations near Frechen,

997 Germany, in: Norwegian Petroleum Society Special Publications. Elsevier, pp. 39–998 50.

299 Lindsay, N.G., Murphy, F.C., Walsh, J.J., Watterson, J., Flint, S., Bryant, I.D.,
1000 1993. Outcrop studies of shale smears on fault surfaces. Geol. Model. Hydrocarb.
1001 Reserv. outcrop Analog. 15, 113–123.

Lisk, M., 2004. Constraints on the oil prospectivity of the Penola Trough,onshore Otway Basin.

Little, B.M., Phillips, S.E., 1995. Detrital and authigenic mineralogy of the
Pretty Hill Formation in the Penola Trough, Otway Basin: implications for future
exploration and production. APPEA J. 35, 538–557.

Liu, Y., Li, H.A., Okuno, R., 2016. Measurements and Modeling of Interfacial
Tension for CO2/CH4/Brine Systems under Reservoir Conditions. Ind. Eng. Chem.
Res. 55, 12358–12375. https://doi.org/10.1021/acs.iecr.6b02446

Lovibond, R., Suttill, R.J., Skinner, J.E., Aburas, A.N., 1995. The
hydrocarbon potential of the Penola Trough, Otway Basin. APPEA J. 35, 358–371.

- 1012 Lyon, Boult, P.J., Hillis, R.R., Mildren, S.D., 2005. Sealing by Shale Gouge
- 1013 and Subsequent Seal Breach by Reactivation: A Case Study of the Zema Prospect,
- 1014 Otway Basin. Eval. fault cap rock seals AAPG Hedb. Ser. no. 2 179–197.
- 1015 https://doi.org/10.1306/1060764H23169
- Lyon, P.J., Boult, P.J., Hillis, R.R., Bierbrauer, K., 2007. Basement controls
 on fault development in the Penola Trough, Otway Basin, and implications for faultbounded hydrocarbon traps. Aust. J. Earth Sci. 54, 675–689.
- 1019 https://doi.org/10.1080/08120090701305228
- Lyon, P.J., Boult, P.J., Mitchell, a, Hillis, R.R., 2004. Improving fault
 geometry interpretation through ' pseudo-depth ' conversion of seismic data in the
 Penola Trough , Otway Basin . 19–22.
- Lyon, P.J., Boult, P.J., Watson, M.N., Hillis, R., 2005. A systematic fault seal
 evaluation of the Ladbroke Grove and Pyrus traps of the Penold Trough, Otway
 Basin. Aust. Pet. Prod. Explor. Assoc. J. 45, 459–476.
- Miocic, J.M., Gilfillan, S.M.V., Roberts, J.J., Edlmann, K., McDermott, C.I.,
 Haszeldine, R.S., 2016. Controls on CO2storage security in natural reservoirs and
 implications for CO2storage site selection. Int. J. Greenh. Gas Control 51, 118–125.
 https://doi.org/10.1016/j.ijggc.2016.05.019
- 1030 Miocic, J.M., Johnson, G., Bond, C.E., 2019. Uncertainty in fault seal
- 1031 parameters: implications for CO 2 column height retention and storage capacity in
- 1032 geological CO 2 storage projects. Solid Earth 10, 951–967.
- 1033 https://doi.org/10.5194/se-10-951-2019
- 1034 Najafi-Marghmaleki, A., Tatar, A., Barati-Harooni, A., Mohebbi, A., Kalantari-
- 1035 Meybodi, M., Mohammadi, A.H., 2016. On the prediction of interfacial tension (IFT)
- 1036 for water-hydrocarbon gas system. J. Mol. Liq. 224, 976–990.
- 1037 https://doi.org/10.1016/J.MOLLIQ.2016.10.083
- 1038 Naylor, M., Wilkinson, M., Haszeldine, R.S., 2010. Calculation of CO 2
 1039 column heights in depleted gas fields from known pre-production gas column
- 1040 heights. Mar. Pet. Geol. https://doi.org/10.1016/j.marpetgeo.2010.10.005

- 1041 Nordgard Bolas, H.M., Hermanrud, C., Teige, G.M.G., 2005. Seal capacity
- 1042 estimation from subsurface pore pressures. Basin Res. 17, 583–599.
- 1043 https://doi.org/10.1111/j.1365-2117.2005.00281.x
- 1044 Øren, P.-E., Bakke, S., 2003. Reconstruction of Berea sandstone and pore-
- scale modelling of wettability effects. J. Pet. Sci. Eng. 39, 177–199.
- 1046 https://doi.org/10.1016/S0920-4105(03)00062-7
- 1047 Pei, Y., Paton, D.A., Knipe, R.J., Wu, K., 2015. A review of fault sealing
- behaviour and its evaluation in siliciclastic rocks. Earth-Science Rev. 150, 121–138.
 https://doi.org/10.1016/j.earscirev.2015.07.011
- 1050 Peng, D.-Y., Robinson, D.B., 1976. A new two-constant equation of state.
- 1051 Ind. Eng. Chem. Fundam. 15, 59–64.
- 1052 Radke, C.J., Kovscek, A.R., Wong, H., 1992. A Pore-Level Scenario for the
- 1053 Development of Mixed Wettability in Oil Reservoirs, in: SPE Annual Technical
- 1054 Conference and Exhibition. Society of Petroleum Engineers.
- 1055 https://doi.org/10.2118/24880-MS
- 1056 Rajayi, M., Kantzas, A., 2011. Effect of Temperature and Pressure on
- 1057 Contact Angle and Interfacial Tension of Quartz/Water/Bitumen Systems. J. Can.
- 1058 Pet. Technol. 50, 61–67. https://doi.org/10.2118/148631-PA
- 1059 Ren, Q.Y., Chen, G.J., Yan, W., Guo, T.M., 2000. Interfacial tension of (CO2
- + CH4) + water from 298 K to 373 K and pressures up to 30 MPa. J. Chem. Eng.
- 1061 Data 45, 610–612. https://doi.org/10.1021/je990301s
- 1062 Rimstidt, J.D., Barnes, H.L., 1980. The kinetics of silica-water reactions.
- 1063 Geochim. Cosmochim. Acta 44, 1683–1699. https://doi.org/10.1016/0016-
- 1064 7037(80)90220-3
- 1065 Robert M. Sneider, J.S.S.G.W.B., Neasham, J.W., 1997. AAPG Memoir 67:
- 1066 Seals, Traps, and the Petroleum System. Chapter 1: Comparison of Seal Capacity
- 1067 Determinations: Conventional Cores vs. Cuttings 1–12.
- Schowalter, T.T., 1974. AAPG bulletin., AAPG Bulletin. AmericanAssociation of Petroleum Geologists.

- 1070 Shipton, Z.K., Cowie, P.A., 2001. Damage zone and slip-surface evolution
- 1071 over μ m to km scales in high-porosity Navajo sandstone, Utah. J. Struct. Geol. 23,
- 1072 1825–1844. https://doi.org/10.1016/S0191-8141(01)00035-9
- Shipton, Z.K., Evans, J.P., Robeson, K.R., Forster, C.B., Snelgrove, S., 2002.
 Structural heterogeneity and permeability in faulted eolian sandstone: Implications
 for subsurface modeling of faults. AAPG Bull. v 86, 863–883.
- Singh, K., Bijeljic, B., Blunt, M.J., 2016. Imaging of oil layers, curvature and
 contact angle in a mixed-wet and a water-wet carbonate rock. Water Resour. Res.
 52, 1716–1728. https://doi.org/10.1002/2015WR018072
- Sperrevik, S., Gillespie, P.A., Fisher, Q.J., Halvorsen, T., Knipe, R.J., 2002.
 Empirical estimation of fault rock properties. Nor. Pet. Soc. Spec. Publ. 11, 109–125.
 https://doi.org/10.1016/S0928-8937(02)80010-8
- 1082Sutjiadi-Sia, Y., Jaeger, P., Eggers, R., 2008. Interfacial phenomena of1083aqueous systems in dense carbon dioxide. J. Supercrit. Fluids 46, 272–279.
- 1084 https://doi.org/10.1016/J.SUPFLU.2008.06.001
- Sutton, R.P., 2006. Oil system correlations. LAKE, LW Pet. Eng. Handbook.Soc. Pet. Eng. 1, 258–306.
- Tassone, D.R., Holford, S.P., Duddy, I.R., Green, P.F., Hillis, R.R., 2014.
 Quantifying Cretaceous–Cenozoic exhumation in the Otway Basin, southeastern
 Australia, using sonic transit time data: Implications for conventional and
 unconventional hydrocarbon prospectivity. Am. Assoc. Pet. Geol. Bull. 98, 67–117.
 https://doi.org/10.1306/04011312111
- Teasdale, J.P., Pryer, L.L., Stuart-Smith, P.G., Romine, K.K., Etheridge,
 M.A., Loutit, T.S., Kyan, D.M., 2003. Structural framework and basin evolution of
 Australia's southern margin. APPEA J. 43, 13–37.
- Tenthorey, E., Dance, T., Cinar, Y., Ennis-King, J., Strand, J., 2014. Fault
 modelling and geomechanical integrity associated with the CO2CRC Otway 2C
 injection experiment. Int. J. Greenh. Gas Control 30, 72–85.
- 1098 https://doi.org/10.1016/j.ijggc.2014.08.021

1099 Tian Yi-Ling, T., Yan-Fan, X., Hong-Xu, Z., Xi-Jing, D., Xiao-Wen, R., Feng-1100 Cai, Z., Yi-Ling, T., Yan-Fan, X., Hong-Xu, Z., Xi-Jing, D., Xiao-Wen, R., Feng-Cai, 1101 Z., 1997. Interfacial Tensions between Water and Non-polar Fluids at High 1102 Pressures and High Temperatures. Acta Physico-Chimica Sin. 13, 89–95. 1103 https://doi.org/10.3866/PKU.WHXB19970120 1104 Treiber, L.E., Owens, W.W., 1972. A Laboratory Evaluation of the Wettability 1105 of Fifty Oil-Producing Reservoirs. Soc. Pet. Eng. J. 12, 531-540. 1106 https://doi.org/10.2118/3526-PA 1107 Vavra, C.L., Kaldi, J.G., Sneider, R.M., 1992. Geological applications of 1108 capillary pressure: a review (1). Am. Assoc. Pet. Geol. Bull. 76, 840-850. 1109 Watson, M.N., Boreham, C.J., Tingate, P.R., 2004. Carbon dioxide and 1110 carbonate cements in the Otway Basin; implications for geological storage of carbon dioxide. APPEA J. 44, 703-720. 1111 1112 Watson, M.N., Zwingmann, N., Lemon, N.M., Tingate, P.R., 2003. Onshore 1113 Otway Basin carbon dioxide accumulations: CO2-induced diagenesis in natural 1114 analogues for underground storage of greenhouse gas. APPEA J. 43, 637-653. 1115 Watts, N.L., 1987. Theoretical aspects of cap-rock and fault seals for single-1116 and two-phase hydrocarbon columns. Mar. Pet. Geol. 4, 274-307. 1117 https://doi.org/10.1016/0264-8172(87)90008-0 1118 Wiegand, G., Franck, E.U., 1994. Interfacial tension between water and non-1119 polar fluids up to 473 K and 2800 bar. Berichte der Bunsengesellschaft für Phys. 1120 Chemie 98, 809-817. https://doi.org/10.1002/bbpc.19940980608 1121 Worden, R.H., Morad, S., 2000. Economic evaluation of a petroleum 1122 accumulation de- mands a Quartz cementation in oil field sandstones: a review of 1123 the key controversies. Spec. Publs int. Ass. Sediment 29, 1–20. 1124 Yielding, G., 2002. Shale Gouge Ratio — calibration by geohistory. Nor. Pet. 1125 Soc. Spec. Publ. 11, 1-15. https://doi.org/10.1016/S0928-8937(02)80003-0

- 1126 Yielding, G., Bretan, P., Freeman, B., 2010. Fault seal calibration: a brief
- 1127 review. Geol. Soc. London, Spec. Publ. 347, 243–255.
- 1128 https://doi.org/10.1144/SP347.14
- 1129 Yielding, G., Freeman, B., Needham, D.T., 1997. Quantitative fault seal1130 prediction. Am. Assoc. Pet. Geol. Bull. 81, 897–917.
- 1131 Ziesch, J., Aruffo, C.M., Tanner, D.C., Beilecke, T., Dance, T., Henk, A.,
- 1132 Weber, B., Tenthorey, E., Lippmann, A., Krawczyk, C.M., 2017. Geological structure
- and kinematics of normal faults in the Otway Basin, Australia, based on quantitative
- analysis of 3-D seismic reflection data. Basin Res. 29, 129–148.
- 1135 https://doi.org/10.1111/bre.12146
- 1136 Ziesch, J., Aruffo, C.M., Tanner, D.C., Beilecke, T., Dance, T., Henk, A.,
- 1137 Weber, B., Tenthorey, E., Lippmann, A., Krawczyk, C.M., 2015. Geological structure
- and kinematics of normal faults in the Otway Basin, Australia, based on quantitative
- 1139 analysis of 3-D seismic reflection data. Basin Res. n/a-n/a.
- 1140 https://doi.org/10.1111/bre.12146