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1 **Oil retention and intrasource migration in the organic-rich lacustrine Chang 7 Shale of the Upper**
2 **Triassic Yanchang Formation, Ordos Basin, Central China**

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18

19 **ABSTRACT:**

20 The Zhang 22 well was drilled in the Ordos Basin, penetrating the Chang 7 Member of the Yanchang
21 Formation, which has more than 80 m cumulative black organic-rich shale of oil window maturity.
22 Utilizing seventy-six samples collected every 1 meter from the well the effects of stratigraphic
23 fractionation and petroleum expulsion within five intervals of the Chang 7 shale were qualitatively
24 and quantitatively documented. The organic-rich intervals-1, -2 and -5, having an average TOC
25 content of 6.79 wt% and pyrolyzable hydrocarbon potential S_2 of 9.40 mg/g rock, are defined as
26 “generative units” in the Chang 7 shale system, compared to the “in-source reservoirs” or “sweet
27 spots” – the third and fourth intervals – which contain lower average TOC content of 4.19 wt% and an
28 average S_2 value of 7.17 mg/g rock, but the highest amount of free oil (av. total oil of 7.35 mg/g rock).
29 Geochemical and molecular compositions display distinctive differences between samples from these
30 source and reservoir groupings. For example, bitumens from the generative units proportionally
31 possess lower saturated hydrocarbons (56% to 66%) than those from the in-source reservoirs (up to
32 81%). The proportions of aromatic and polar compounds in the generative units are accordingly
33 higher than in their counterpart. The individual molecular weight distribution of sample extracts
34 displays more light-end moieties being enriched in the generative units. By applying the
35 compositional mass balance calculation, the overall and compound-specific expulsion efficiencies in
36 the in-source reservoirs are abnormally negative compared to the positive values in the generative

37 intervals. This finding in conjunction with the effects of the preferential retention of aliphatic
38 hydrocarbons and the differential expulsion of light molecular weight compounds in the in-source
39 reservoirs together indicate a short-distance intrasource migration of generated petroleum into the
40 sweet spot intervals (intervals-3 and -4) from the overlying units (intervals-1 and -2) and the
41 underlying interval-5. Furthermore, when quantifying the total amount of retained petroleum in the
42 shale system, an amended assessment has been introduced to overcome the systematic
43 misestimations if only unextracted S_1 values were considered. Thus, the oil crossover effect, T_{\max} shift
44 phenomenon and the HI being shifted to higher values after extraction all account for identifying the
45 intervals-3 and -4 as the in-source reservoirs. In this study, we have not only identified a set of
46 promising in-source target for shale oil exploration and production, but we also presented the
47 chemical and molecular composition for these shale oils. We have additionally speculated for the
48 intrasource migration model, and further discussed the different expulsion efficiencies in the shale
49 system upon the compositional mass balance calculation, and the stratigraphic fractionation on
50 differentiating the chemical compositions during migration. The improved oil quality by fractionation,
51 the extra storage potential derived from microfossil quartz, the weak adsorptive affinity of oil to
52 organic matter, and the good shale frackability all give a promising prospective for exploring and
53 producing shale oil from the Chang 7 shale system in the Ordos Basin.

54 **Keywords:** retention; expulsion efficiency; intrasource migration; mass balance calculation;

55

56 1. Introduction

57 The shale oil system has been defined as organic-rich mudstone units in which the generated oil is
58 retained in-place, or has migrated into closely juxtaposed organic-lean rocks (Jarvie, 2012). The term
59 hybrid has also been used to describe production from the organic-lean intervals (Welker et al., 2013)
60 within tight oil plays (Jarvie, 2014). In China, the tight shale and the juxtaposed tight sandstone plays
61 have been assigned as belonging to two different kinds of petroliferous accumulations, namely those
62 with the in-situ subsurface matrix permeability lower than $0.001 \times 10^{-3} \mu\text{m}^2$ (0.001 mD) (China-
63 National-Standard, 2015) and $0.1 \times 10^{-3} \mu\text{m}^2$ (0.1 mD) (China-National-Standard, 2014), respectively. In
64 the current communication, shale oil refers to liquid hydrocarbons preserved in muddy or shaly rocks
65 (e.g. mudstone, shale), whereas tight oil is assigned by this study to hydrocarbons stored in sandy
66 deposits, such as siltstone and fine sandstone.

67 As an important non-marine petroliferous basin, the Ordos Basin contains oil and natural gas
68 resources that amount to nearly one third of China's annual gross output (Yang and Deng, 2013)
69 (Figure 1). It has been reported that by the end of 2015, the proven total petroleum reserves in the
70 Ordos Basin are over 4.00×10^9 t (2.92×10^{10} bbl) of oil (PetroChina, 2016b) and 3.27×10^{12} m³ ($1.15 \times$
71 10^{14} ft³) of natural gas (Yang et al., 2012; Zou et al., 2013). Additionally, up to 2.43×10^7 t (1.77×10^8
72 bbl) of oil and 3.47×10^{10} m³ (1.22×10^{12} ft³) of natural gas have been produced from the Ordos Basin
73 in 2013 annually, which makes it the biggest petroleum producer in China with an annual production

74 of more than 5.20×10^7 t (3.79×10^8 bbl) (Yang et al., 2016a). The Upper Triassic Yanchang Formation
75 has been determined to be the effective source rock for charging the Mesozoic conventional
76 petroleum accumulations in the Ordos Basin (Zhai, 1997; Hanson et al., 2007; Ji et al., 2007; Duan et
77 al., 2008; Yu et al., 2010), and it also has been defined as a self- sourced and preserved petroleum
78 system containing oil and gas in ultra-tight fine-grained rocks (Yang et al., 2012; Zou, 2013; Zou et al.,
79 2013; Yang et al., 2016b; Yang et al., 2016d) (Figure 2).

80 Many studies have been focused on the reservoir features of tight oil or shale oil, such as sandbody or
81 shale distribution (Fu et al., 2013; Yao et al., 2013), mineralogical composition (Xu et al., 2013), time
82 of oil accumulation (Yao et al., 2013) and resource potential (Yang et al., 2013; Yang et al., 2016b).
83 Although others have characterized the chemical composition of the produced crude oil from the
84 Yanchang Formation, their interests have been mainly focused on source-oil correlation, or on the
85 reservoired liquids in the ultra-tight thin sandstone, rather than on the bitumen retained in purely
86 shaly intervals. For example, by examining the *n*-alkane chain length distribution, ratios of tricyclic and
87 tetracyclic terpanes and the abundance of C₂₉ sterane of crude oils from the Xifeng Oilfield, Duan et al.
88 (2008) found that the investigated oils were generated from a mixed source of terrigenous and algal-
89 bacterial organic matter. These oils are of low sulphur content, low density, low viscosity and freezing
90 point, all of which favors high liquid mobility (Yao et al., 2015).

91 When considering the compositional relationships between bitumen in source rocks and petroleum in
92 reservoirs, a fundamental difference was first observed by (Brenneman and Smith Jr (1958);
93 Moldowan et al., 1985). The oils produced from the host reservoirs are enriched in saturated
94 hydrocarbons, whereas the bitumen extracts from shale are asphaltenes- and resins-rich (Pelet and
95 Tissot, 1971). This phenomenon has been ascribed to be a consequence of stratigraphic fractionation
96 during expulsion and migration, and the aliphatic compounds are more preferentially expelled over
97 aromatic hydrocarbons, which leaves more polar fractions behind in the source rocks (Baker, 1962;
98 Thompson and Eglinton, 1978). Otherwise, physical fractionation has also been reported as having
99 taken place so that smaller size molecular components are preferentially expelled relative to larger
100 ones (Mackenzie et al., 1983; Leythaeuser et al., 1984; Leythaeuser et al., 1988; Esemé et al., 2007).
101 The centimeter-scale intraformational migration within tight stratigraphic packages would also bring
102 about fractionation in unconventional shale systems (Jarvie, 2014), which gives rise to differing
103 chemical signatures in bitumens (Bernard et al., 2012; Bernard and Horsfield, 2014).

104 Although some researchers have recognized the geochemical differences between crude oils and
105 source rock extracts in the petroliferous Yanchang Formation (Hanson et al., 2007; Tao et al., 2015; Ji
106 et al., 2016; Yang et al., 2016c), few of them have quantitatively examined the compositional and
107 molecular differences, utilizing compositional mass balance calculations. Furthermore, elucidating the
108 controlling factors on the bulk gas-to-oil (GOR) of shale oil, the effects of intraformational retention
109 and fractionation on chemical composition are significant, because with the pressure drawdown
110 during production even subtle changes in bulk fluid composition would bring about large difference in

111 phase envelope geometry (Han et al., 2015), and these issues have yet to be addressed for the Ordos
112 Basin.

113 Thus, in this paper, we first present the bulk mineralogical composition and lithofacies of Chang 7
114 shale to characterize its inorganic composition. Then the organic properties, such as bulk organic
115 matter characteristics, types and macromolecular structure, are examined to reveal the quality of
116 source rocks and the capacity for generating hydrocarbons during maturation. Furthermore, we focus
117 on making a prediction on petroleum types through the whole thermal history, characterizing the
118 geochemical composition of retained petroleum, as well as assessing the compositional mass balance.
119 Based on these results, we have been able to quantify the generated, retained and expelled amounts
120 of hydrocarbons during maturation, and consequently calculate the expulsion efficiency of individual
121 *n*-alkanes for each sample. Thereafter, we were able to assess the inorganic and organic controls,
122 namely minerals and kerogens, on hydrocarbons storage in the Chang 7 shale, as well as establishing a
123 hydrocarbon generation-retention-expulsion model.

124 2. Geological Background

125 The Ordos Basin is an intraplate depression on the North China Craton formed during the Mesozoic to
126 Cenozoic in central China (Figure 1-a) (Liu et al., 2008; Wan et al., 2013), and is bounded by a series of
127 synchronous, polyphase orogens, i.e. the Yishan Orogen to the north, the Lvliang Orogen to the east,
128 the Qinling to the south and the Liupan-Helan Orogens to the west (Yang et al., 2005; Wan et al.,
129 2013). The Liupan orogenic activity deformed the southwestern Ordos Basin, resulting in several
130 foreland depressions (Liu and Yang, 2000). The basin can be subdivided into six regional structural
131 units (Figure 1-b).

132 Upper Triassic non-marine clastic rocks records sedimentation within the basin, and is continuously
133 distributed from the Tianhuan Depression to the Yishan Slope (Figure 1-c). These sediments
134 unconformably overly the Middle Triassic Zhifang Formation, and is unconformably overlain by the
135 Lower Jurassic Fuxian Formation (Figure 2). The sediments of the Yanchang Formation, the chief
136 source for conventional petroleum in the basin, are composed of fluvial sandstone, siltstone, shallow
137 lacustrine mudstone and deep lacustrine, laminated black shale. Yellowish tuff intervals are
138 interbedded within the Yanchang sediments varying from 0.2 to 0.45 cm (0.08 to 0.18 in) (Qiu et al.,
139 2014). The overall thickness of the Yanchang sedimentary package is 800 to 1000 m (2624 to 3281 ft)
140 in the north, and gradually thickens southward to 1000-1400 m (3281 to 4593 ft) (Pan et al., 2016).
141 Using important marker beds, sedimentary cycles and lithological combinations, the Yanchang
142 Formation has been subdivided into ten members by the Changqing Oilfield Company of PetroChina
143 (COCP), named Chang 1 to Chang 10 (Figure 2). The Chang 7 Member is the most prolific source
144 interval, mainly consisting of organic-rich black, laminated shale that is rich in oil-prone organic
145 matter derived from acritarchs (*Leiosphaeridia* sp.), as well as some *Botryococcus* (Ji et al., 2008; Ji et
146 al., 2010). Chang 7 is further subdivided into three units according to the stratigraphic category of the
147 COCP based on lithology, i.e. Chang 7-1, Chang 7-2 and Chang 7-3 (Figure 2).

149 **3. Materials and Methods**

150 **3.1. Sample Set**

151 A suite of 76 core samples were retrieved at regular 1-m intervals across 1538.30 – 1605.60 m
152 (5046.90 – 5267.7 ft) from the Upper Triassic Yanchang Formation of the Zhang 22 well (see well
153 location in [Figure 1](#)). Most of these samples were black shales or dark grey mudstones, only eight light
154 grey siltstones were found in the uppermost part of the well. Note that two siltstones were collected
155 from the Chang 6 Member, whereas the remaining six samples were obtained from interval-1 of the
156 Chang 7-1 unit. In addition to the Zhang 22 well samples, one immature shale (G014952, containing
157 Type-I kerogen) of the Chang 7 shale from a previous study was used as a reference in the mass
158 balance calculation. The reader is referred to Pan et al. (2016) for a detailed geochemical
159 characterization of this sample.

160 **3.2. Thin Section Microscopy**

161 Samples were mechanically polished into 0.03 mm (0.001 in) thin sections parallel (20 slices) and
162 perpendicular (20 slices) to the bedding. Then, by applying transmitted white light, reflected white
163 light and blue-light fluorescence (fluorescence excitation wavelength band 350-420 nm) microscopy
164 using a Zeiss Axioplan microscope, thin sections were analyzed to reveal fabric and texture of fine-
165 grained shales and organic-inorganic relationships. Immersion oil (refractive index of 1.515) and oil
166 immersion objectives were employed to increase the resolving power of the microscope.

167 **3.3. Rock-Eval Pyrolysis and Total Organic Carbon Determination**

168 Rock-Eval parameters were measured on all 76 samples using a Rock-Eval 6 Instrument following the
169 standard technique described by (Espitalie et al., 1977; Lafargue et al., 1998; Behar et al., 2001) with a
170 programmed temperature system from 300 °C (572 °F, 3 min) to 650 °C (1202 °F, 0 min) at 25 °C (77 °F)
171 per min. Jet-Rock 1 was run as every tenth sample and checked against the acceptable range given in
172 the Norwegian Industry Guide to Organic Geochemical Analyses (NIGOGA, 2000). After mixing the
173 finely powdered rock samples with dilute (10% vol) HCl at 60 °C ± 5 °C (140 °F ± 41 °F) for 1 hour to
174 remove carbonate, all samples were washed using distilled water to remove all traces of HCl and
175 water-soluble chlorides. The concentration of total organic carbon was measured as carbon dioxide
176 with infrared (IR) detector in an oxygenated combustion oven up to 1350 °C (2462 °F) using a LECO SC-
177 632 apparatus. Twenty samples were randomly selected from each interval to be subjected to solvent
178 extraction (discussed below), and then measured again.

179 3.4. Thermovaporization Gas Chromatography (Tvap-GC) and Pyrolysis Gas Chromatography (Py- 180 GC)

181 Thermovaporization gas chromatography (Tvap-GC) was performed on 76 samples to characterize the
182 free hydrocarbons. Twenty-six mm long capillary glass tubes (an internal diameter of 3 mm [0.12 in])
183 with both open ends were preheated at 600 °C (1112 °F) for no less than 1 h to remove contaminants.
184 After that, up to 30 mg (0.001 oz) untreated and powdered sample were positioned in the center of
185 the glass tube using glass wool. Then, the glass tube was sealed and inserted in the holder of the
186 temperature-programmed oven of the Quantum MSSV-2 Thermal Analysis System (Horsfield et al.,
187 1989; Horsfield et al., 2015). The tube was heated in a flow of helium up to 300 °C (572 °F) for 5 min to
188 purge outside contaminants. After heating at 300 °C (572 °F) for 10 min, the tube was crushed and the
189 products were liberated and transferred into an Agilent GC-6890A gas chromatography.

190 Afterward, the temperature of the oven was raised up to 600 °C (1112 °F) from the initial 300 °C
191 (572 °F, maintaining for 2 min) at a speed of 50 °C/min (122 °F/min) to continue the open-system
192 pyrolysis gas chromatography (Py-GC) for characterizing the macromolecular structure of labile
193 kerogen. Pyrolysates were collected using a liquid nitrogen-cooled cryogenic trap (at -196 °C [-320 °F]),
194 and injected into an Agilent GC-6890A by ballistic heating (holding at 300 °C for 10 min) for gas
195 chromatographic analysis (HP-Ultral, 50 m × 32 mm [164 ft × 1.26 in] i.d., dimethylpolysiloxane-coated
196 column with 0.52 µm film thickness). Individual compounds and boiling ranges (C₁, C₂₋₅, C₆₋₁₄ and C₁₅₊)
197 were quantified with reference to *n*-butane external standard by peak area integration (ChemStation
198 Software © Agilent Technologies).

199 3.5. Extraction and Fractionation

200 Roughly 30 g of each of the 76 powdered samples were extracted using a ternary azeotropic solvent
201 system (vol. % acetone : chloroform : methanol = 38 : 32 : 30) for 24 h at 60 °C (140 °F) using a Soxhlet
202 extraction apparatus. After extraction, selected extracts (15) were separated into maltenes (*n*-
203 hexane-soluble fraction) and asphaltenes according to the precipitation method described by
204 Theuerkorn et al. (2008). The *n*-hexane-soluble fractions (maltenes) were further subjected to
205 medium pressure liquid chromatography (MPLC) to separate into saturated, aromatic hydrocarbons
206 and resins (Radke et al., 1980). All aforementioned measurements were performed in the Organic
207 Geochemistry Laboratory of Deutsches GeoForschungsZentrum (GFZ).

208 3.6. Reference dataset

209 A reference dataset from our previous work is cited here to provide additional information for the
210 Chang 7-3 unit due to the omission of core collection for the Zhang 22 well. Detailed description of
211 sample set and experimental methods, as well as geochemical and molecular characterizations can be
212 inferred from Pan et al. (2016).

213 4. Results

214 4.1. Subdividing Scheme

215 [Figure 3](#) shows a good subdividing scheme for the Chang 7 shale from the Zhang 22 well according to
216 the mineralogical composition, bulk Rock-Eval parameters and soluble extract yields. The investigated
217 succession can be subdivided into five intervals ([Table 1](#)). Intervals-1 and -2 equal to the Chang 7-1
218 unit, and show a relatively high content of organic matter up to 14% and high S_2 values. Intervals-4
219 and -5 represent the Chang 7-2 unit, and contain lower TOC content with respect to that in the upper
220 part of succession. Interval-3, interbedded in the middle of Chang 7-1 and Chang 7-2 units, is
221 characterized by the relatively lowest TOC content and the highest hydrogen index, OSI values and
222 extractable yields compared to other intervals, which make it greatly unique among all five intervals.
223 More detailed work need to be considered to explain this difference between interval-3 and others. In
224 addition, a reference dataset from our previous work is cited here to provide additional information
225 for the Chang 7-3 unit (Pan et al., 2016). Some samples share particularly lithological, mineralogical,
226 geochemical and molecular similarities which make them appear to be associated with a specific
227 population ([Table 1](#)).

228

229 4.2. Bulk Mineralogical Composition

230 [Figure 3](#) shows the bulk mineralogical composition of the Zhang 22 well as a function of depth. It
231 reveals a strong and systematic depth-dependent heterogeneity, though the entire investigated
232 succession is merely composed of two distinctive types of lithology. In general, a compensatory
233 relationship between brittle minerals (i.e. quartz plus feldspar) and clay minerals can be observed; the
234 higher the content of brittle minerals, the lower the content of clay minerals. The carbonate content
235 is extremely low (overall av. 2.93%) throughout the entire succession, and the terrigenous clastic
236 minerals make the predominant contribution to the bulk mineralogical composition ([Table 2](#)). For the
237 eight siltstone samples (two of Chang 6 and six from interval-1), clay minerals only amount to an
238 average percentage of 23.50, and the mineral composition is predominantly determined by quartz
239 and feldspar (av. 31.20% and 35%, respectively).

240 Clay minerals become the dominant component (>40%) through interval-1 to interval-5 (a detailed
241 description of subdivision for entire succession will be presented latter), yet they show a decreasing
242 then increasing trend at the bottom of interval-1. With increasing burial depth, the content of clay
243 minerals approaches a uniform distribution ([Figure 3](#)), but the average values for each interval
244 through interval-1 to interval-4 are elevated (from 41.02% to 52.15%), and then slightly decrease to
245 51.11% in interval-5 ([Table 2](#)). Similar to the clay minerals, the distribution of feldspar varies
246 significantly in the first interval, and shows a mirror image relative to the clays throughout the whole
247 succession ([Figure 3](#)). This variation is partially attributable to the presence of siltstones interbedded
248 in the black shale interval, because the content of feldspar in siltstones (35.00%) is higher than in the

249 remaining five intervals (av. 24.92%). The distribution of feldspar through interval-2 to interval-5
250 displays a much more consistent pattern than clay minerals do and accordingly, decreases from
251 interval-1 (29.97%) to interval-4 (21.54%), and then increases to 22.28% in interval-5 (Table 2). The
252 scenario for quartz is a little more complicated than for the other two mineral components, however,
253 it still shows a generally negative correlation to clay content (Figure 3), and presents low contents
254 with respect to feldspar (Table 2). Quartz again, is scattered in interval-1, since the content in
255 siltstones (31.19%) is much higher than that in shales (average value among five intervals of 18.86%).
256 From interval-1 to interval-5, quartz is distributed more uniformly with a relatively low average value
257 of 20.26% compared to feldspar. Pyrite is presented throughout the whole succession (av. 7.08%),
258 and accounts for similar values in each interval apart from the siltstones (Table 2).

259 Figure 4 shows the relative amounts of clay minerals, carbonate and quartz. Here again, siltstones are
260 excluded from interval-1, and intentionally displayed by different symbols in order to make a
261 meaningful discussion of lithological types. Almost all samples contain low carbonate content, less
262 than 20%, and then can be further grouped to two populations according to the relative amount of
263 quartz and clay minerals. Most of siltstones and samples from interval-1 combining with two Chang 6
264 siltstones are composed of quartz more than 40%. This population can be described as siliceous. Note
265 that a sample from interval-2 has been grouped into this population because it locates adjacently to
266 the bottom of interval-1. In contrast, all samples from the intervals-2, 3, 4, 5 as well as partial
267 siltstones and that from interval-1 are characterized by a clay content exceeding 60%. These are
268 defined as argillaceous. The first interval again, shows a significant heterogeneity in mineral
269 composition, even when siltstones are excluded. The remaining samples display a uniform
270 distribution when considering the relative content of clay minerals, carbonate and quartz.

271 4.3. Sedimentary Stratigraphy and Lithofacies

272 The investigated section of the Yanchang Formation consists primarily of profundal laminated shale
273 and occasional grey mudstone and siltstone interbeds, which together represent an organic-rich
274 lacustrine succession (Table 1). The overlying Chang 6 Member and the underlying Chang 8 Member
275 are composed of fining-upward deltaic fine-grained sandstones (Liu et al., 2014; Yuan et al., 2015; Pan
276 et al., 2016), the entire Chang 7 Member shows a strong lithological homogeneity of shale suggesting
277 a lack of distinctive cyclicity and a continuous, stable depositional environment (Figure 2). However,
278 from the massive lake expansion in the Chang 7-3 to the shoaling upwards in the Chang 7-1, general
279 lake-level fluctuations can be recognized in three stages: rapid expansion, persistent drawdown and
280 slow elevation (Pan et al., 2016). In addition, there is no obvious sign of subaerial exposure or the
281 presence of evaporite deposits in the Chang 7 shale.

282 The first interval of the Chang 7 shale was formed during lake shrinkage, and some deltaic front
283 siltstones are interbedded within homogeneous shales (Yuan et al., 2015). Eight siltstone layers no
284 thicker than 1 m (3.28 ft) are observed in the Chang 6 and interval-1 (Figure 5-a). The remaining
285 samples are laminated shales containing planar laminae substantially less than 1 mm (0.04 in) thick

286 (Figure 5-b and d). The presence of pyrite usually appears in the shale samples from interval-1 (Figure
287 5-c).

288 The shaly interval-2 was mainly deposited under a profundal lacustrine environment, and appears as
289 massive laminated black shales in core. Laminae of organic-matter are shown in photomicrographs
290 (Figure 5-e), and individual lacustrine alginite containing bitumen can be identified under the blue-
291 light excitation (Figure 5-f and g). Pyrite is also present in this interval (Figure 5-h). This argillaceous,
292 non-calcareous and pyrite-containing shale facies ascribe interval-2 to a low energy, anaerobic
293 depositional environment dominated by suspension settling.

294 The argillaceous intervals 3, 4 and 5 are also composed of laminated shale (Figure 5-i, l and m). The
295 lack of sedimentary structures in the core samples indicate a prevailed euxinic depositional
296 environment below the minimum oxygen layer, which is responsible for high amounts of organic
297 matter and clay minerals in these intervals. Pyrite can be observed in the shale (Figure 5-j, k and n),
298 and some terrigenous organic matter notably fusinite are shown in G016091 from interval-3 (Figure 5-
299 j). The majority of the organic matter appears as amorphous forms dispersed in the argillaceous
300 matrix (Figure 5-o).

301 4.4. Bulk Organic Matter Characterization

302 Figure 3 presents the geochemical profiles that are the basis for subdividing the studied Chang 7
303 succession into five intervals.

304 The temperature at which the rate of S_2 generation is at maximum (T_{max}) provides insights into the
305 maturity of kerogen (Espitalie et al., 1977; Tissot and Welte, 1980, 1984; Peters, 1986), though other
306 factors come into play in intercalated source and reservoirs (Han et al., 2015). With the exception of
307 eight siltstone samples, the T_{max} values of investigated shales are commonly between 422 and 472 °C
308 (791 and 881 °F) with an average of 455 °C (851 °F). This broad range, covering the entire oil window
309 (Peters, 1986), clearly does not simply reflect the influence of thermal maturity because of the
310 restricted depth interval under evaluation, and the inhomogeneous distribution of values. Samples
311 from interval-1 and -2 have roughly identical T_{max} values distribution (456°C [852 °F] for interval-1 and
312 459°C [858 °F] for interval-2). The average value for the siltstones is extremely low (335.38 °C
313 [635.68 °F], Table 3) and reflects the presence of involatile bitumen components rather than kerogen.
314 In interval-3, T_{max} is uniformly low, with an average value of 437 °C (818 °F), this being much lower
315 than the overlying and underlying intervals (Figure 3). From interval-4 to interval-5, the T_{max} values
316 are higher again, being 456 and 463 °C (852 and 865 °F), respectively. The causes for the variations in
317 T_{max} are discussed below. As regards the influence of maturation, it should be noted that samples
318 from Chang 7-3 have a T_{max} of 446 °C (834 °F) at the early stage of oil window, in line with a Type I
319 kerogen signature (Pan et al., 2016).

320 Although the content of total organic carbon is generally high, up to a maximum value of 14 wt. %
321 with an overall average value of 5.33 wt. %, the pre-maturation values of TOC were higher due to the

322 present level of maturity. As mentioned before, interval-1 shows heterogeneity due to the presence
323 of siltstones. As expected, the average TOC of eight siltstone samples is quite low (0.85 wt%). These
324 siltstones from the Chang 6 and interval-1, therefore, can be assigned into the Population I. The
325 remaining samples in interval-1 exhibit an average TOC content of approximately 5.89 wt% (Table 3).
326 The highest average TOC content (8.73 wt%) appears in interval-2 with the highest average
327 hydrocarbon generative potential as well ($S_2 = 12.77$ mg/g rock). The values gradually decrease with
328 increasing depth. S_2 shows the same trend too, approaching the lowest value at the lowermost of
329 interval-2. Consequently, samples from the first and second intervals have been assigned as the most
330 organic-rich population (i.e., Population II) in the investigated succession. The third interval is the
331 leanest, with an average TOC content of 3.56 wt%. No obvious variation of TOC values is present in
332 interval-3, and the same applies to S_2 . The average petroleum generative potential S_2 for interval-3 is
333 also the lowest (6.91 mg/g rock). The TOC content and S_2 average value in interval-4 are both higher
334 than in the overlying interval-3 reaching 4.82% and 7.43 mg/g rock, respectively (Table 3). Samples
335 from these two intervals have been classified into the Population III. In interval-5, the TOC values
336 display a similar distribution pattern to interval-4, with an average of 5.77 wt%. The generative
337 potential S_2 varies very little, with an average value only slightly lower than interval-4's (7.36 mg/g
338 rock). In addition, the reference dataset shows that the Chang 7-3 shale has extremely high TOC
339 contents (av. 10.98 wt%) and S_2 values (av. 38.61 mg/g rock) compared to Zhang 22 well (Figure 3 and
340 Table 3). Therefore, shales from this unit could be assigned as the most prolific population in the
341 entire Chang 7 Member (Pan et al., 2016).

342 Figure 6 shows the petroleum potential in the Zhang 22 well using pyrolyzable products (S_2) versus
343 total organic carbon (TOC). All samples generally fall along a regression line of 150 mg HC/g TOC
344 hydrogen index (HI). This distribution represents the remaining generative potential of Type I
345 kerogens at the oil window maturity (Langford and Blanc-Valleron, 1990), which will be fully discussed
346 later (Figure 7). Hydrogen indices in interval-1 display an obvious variation (Figure 3), and show a
347 relatively uniform average value of 135.88 mg/g TOC when excluding the siltstone samples (Table 3).
348 The HI values are slightly enhanced in the second interval (av. 144.73 mg HC/g TOC) and then, reach
349 the highest value of 194.63 mg HC/g TOC in the third interval. After that, the average values gradually
350 decrease to 156.67 mg HC/g TOC in interval-4, and further decline to 129.08 mg HC/g TOC in the
351 lowermost part of the Zhang 22 well (Figure 3 and Table 3). Furthermore, Chang 7-3 samples from the
352 reference dataset denote a notably high value of hydrogen index up to 365.45 mg HC/g TOC,
353 approximately 2.5 times to the overall average of non-siltstone samples, which are also shown in the
354 Figure 6. This difference of generative nature between Chang 7-3 and the combination of Chang 7-1
355 and 7-2 might be attributable to the different kerogen types, in which Chang 7-3 is tending towards
356 Type-I kerogen, while Chang 7-1 and 7-2 are principally Type-II kerogen (Figure 7).

357 Oxygen indices (OI) in interval-1 show widely dispersed points due to the lithological heterogeneity of
358 this interval (Figure 3). With increasing depth OI values tend to be uniform with an average value of
359 5.27 mg CO₂/g TOC for interval-2 and then, rise to 9.50 mg CO₂/g TOC in interval-3. Right after that
360 they slightly drop down to the values of 7.42 and 6.54 mg CO₂/g TOC in the intervals-4 and 5,

361 respectively. Our reference dataset also indicates an OI distribution pattern for the Chang 7-3 Shale
362 addressing a low average value of 4.55 mg CO₂/g TOC similar to the overall pattern in this study
363 (Table 3).

364 4.5. Organic Matter Type and Macromolecular Structure

365 Figure 7 shows kerogen typing on a pseudo van Krevelen diagram and a T_{max} versus hydrogen index
366 diagram. From both diagrams siltstones are clustered apart from the domain area of shales. The
367 relatively high maturation level at the oil window makes it difficult to successfully discriminate the
368 kerogen type based on Rock-Eval-derived generative potential parameters. In Figure 7-a, samples are
369 gathered at the converging maturation pathways where the hydrogen index versus oxygen index
370 diagram is no longer effective to differentiate kerogen types. Samples from Chang 7-3, however,
371 containing higher hydrogen indices seem to imply a highly oil-prone Type I kerogen (Peters, 1986;
372 Delvaux et al., 1990; Behar et al., 2001). Figure 7-b indicates a better grouping pattern for shales, in
373 which although interval-1 always displays a greater scatter, all samples lie between 0.5 and 1.3 % R_o
374 in the Type-I and II kerogen domain. Those from Chang 7-3 are much closer to the Type-I domain
375 showing different organic matter in nature from studied shales (Pan et al., 2016).

376 Py-GC provides more detailed insights into organic matter type in terms of macromolecular structure,
377 utilizing *n*-alkenes, phenol and aromatic hydrocarbons (Figure 8). Phenol-poor type kerogens can be
378 distinguished in Figure 8-a inferring very low amounts of land-plant-derived moieties involved in the
379 kerogen structure and a maturity greater than R_m = 1.6% (Larter and Horsfield, 1993). Chang 6 and
380 interval-1 samples carry more terrestrial origin moieties inferred by a relatively high proportion of *m*,
381 *p*-xylene content, yet most of the shales from the remaining intervals are plotting closer to the *n*-
382 octene apex indicating aquatic organic matter origins of mixed Type-I and II kerogens. In addition,
383 since pyrolytic thiophenes have proportional relationships with kerogen-bond-sulphur molecules
384 (Eglinton et al., 1990), Figure 8-b allows discrimination of kerogen types with high sulphur content
385 deposited in marine environments, and those kerogens structurally dominated by aliphatic moieties
386 from lacustrine settings or by aromatic pyrolysates in terrigenous environments (Mahlstedt and
387 Horsfield, 2012). Higher aromaticity illustrated by high ratios of *o*-xylene to *n*-nonene can be observed
388 in most of samples from the Chang 6 and interval-1, whereas the rest of studied samples lie in the
389 intermediate zone suggesting Type-II kerogens. The dominant proportion of aliphatic over aromatic
390 compounds is released in the form of labile moieties from the non-condensed structure of Type-II
391 kerogen during artificial and natural thermal evolution (Behar and Vandenbroucke, 1987).

392 4.6. Predicted Petroleum Type

393 Py-GC data was further employed for characterization of chain length distribution and prediction of
394 petroleum generative organofacies (Horsfield, 1989, 1997). By calculating the relative amounts of
395 different aliphatic moieties i.e., the sum of C₁₋₅ total hydrocarbons, the sum of C₆₋₁₄ *n*-alkanes and *n*-
396 alkenes as well as the sum of C₁₅₊ *n*-alkanes and *n*-alkenes in pyrolysates, five predicted organofacies

397 can be identified in [Figure 9](#) in close relation to the petroleum classification nomenclature of (Tissot
398 and Welte, 1984; Horsfield, 1997).

399 Two Chang 6 siltstones are dominated by short to moderate chain length distributions (usually less
400 than C₁₄), and exhibit paraffinic-naphthenic-aromatic (PNA) low wax petroleum type organofacies
401 pyrolytic compositions ([Figure 9](#)). However, the heterogeneous first interval has different generative
402 petroleum types. For example, some samples share the same organofacies with Chang 6 siltstones,
403 containing higher amounts of long straight-chain aliphatic precursor materials; while others, including
404 siltstones from interval-1, generate pyrolytic products of gas and condensate that have more lower
405 molecular weight moieties and less C₅₊ normal hydrocarbons ([Figure 9](#)). The heterogeneous nature of
406 interval-1 is closely related to the configuration of molecular structures, inferring a PNA low wax
407 petroleum type grading into the gas and condensate facies. This nature of heterogeneity is also
408 supported by the widely distributive range of relative ratios of aromatic hydrocarbons over *n*-alkenes
409 (i.e., *m*, *p*-xylene over *n*-octene and *o*-xylene over *n*-nonene, [Figure 8-a and 8-b](#)) (Larter, 1984b;
410 Eglinton et al., 1990). Besides, [Figure 9](#) shows the present day signature so that lower maturity
411 samples might have a waxy oil potential (Horsfield, 1989, 1997).

412 The remaining investigated samples are characterized by pyrolysates enriched in short and
413 intermediate alkyl-chains compared to gas compounds, suggesting PNA low wax oil generation in
414 nature ([Figure 9](#)). Only one outlier from interval-3 is located in the paraffinic oil domain with a high
415 wax content. This kind of petroleum generative nature is enriched in paraffinic oil with high wax
416 content, presumably formed by the cracking of long and intermediate alkylated structure. All of
417 samples from cited Chang 7-3 unit yield pyrolysates with a paraffinic high wax oil potential, owing to
418 an aquatic organic matter origin of a mixed Type-I and II kerogen which is supported by the extension
419 of doublets of long chain *n*-alkane and *n*-alkene homologues up to C₃₀ upon the pyrolysis gas
420 chromatography approach (Pan et al., 2016).

421 **4.7. Geochemical Composition of Retained Petroleum**

422 The gross composition of extracts can be defined by the content of maltenes and asphaltenes, in
423 which the former fractions consist of aliphatic (saturated) hydrocarbons, aromatic hydrocarbons, and
424 resins. [Figure 10](#) shows the proportional composition of the maltenes fraction. Extracts of siltstones
425 from Chang 6 and the first interval were calculated together not only because of their identical
426 lithology but they also share similarities in bulk organic matter characterization and macromolecular
427 structure. For siltstones and other shales from five intervals, two classes can be differentiated
428 regarding the relative proportions of aliphatic group of components by greater than or less than 75%.
429 For example, extracts from siltstones, intervals-3 and -4 have aliphatic fraction greater than 75%,
430 followed by resins in proportion (less than 13%) and then, the aromatics (no greater than 11%). By
431 contrast, the bitumens from intervals-1, -2 and -5 contain only approximately 56% – 66% saturated
432 hydrocarbons, and are relatively enriched in aromatic hydrocarbons up to ~20%, and polar
433 compounds that amount to nearly 19% – 24%. The average extraction yields of aliphatics from

434 siltstones as well as shales in the intervals-3 and -4 are normally greater than 0.90 mg/g rock,
435 compared with that in interval-2 and 5 (0.70 and 0.68 mg/g rock, respectively, [Table 4](#)). Although the
436 average aliphatic yield in interval-1 is 1.11 mg/g rock (greater than 0.90 mg/g rock), the contents of
437 aromatic compounds and resins in it are similar to those from intervals -2 and -5 characterized by
438 average amounts of aromatic and resins more than 0.20 mg/g rock ([Table 4](#)). The average amounts of
439 these two fractions, however, seldom reach 0.17 mg/g rock in siltstone samples and shales of interval-
440 3 and -4.

441 The T_{vap}-GC-derived compositional distributions of *n*-alkanes are individually presented in histograms
442 for each interval ([Figure 11](#)). The depletion of gas components from C₁ to C₅ is mainly caused by
443 sample preparation. Short-chain length molecules (C₅₋₁₀) play a dominant role in *n*-alkanes
444 distributions of thermal extracts from the most organic-rich interval-1 and interval-2. They have the
445 same carbon number preference C₈. The contents of the specific carbon molecules increase among
446 short-chain range reaching up to C₈ and then, gradually decrease with the increasing of carbon
447 numbers. Samples from these two intervals are clustered to form the Population II in [Figure 12](#). Short-
448 intermediate chain length *n*-alkanes dominate the fifth interval, which has the main carbon number of
449 C₁₀ slightly higher than that in samples with dominance of short-chain length molecules. These
450 extracts from interval-5 are also classified into the Population II. Otherwise, thermal extracts from
451 siltstones, interval-3 as well as interval-4 are dominated by intermediate-chain (C₁₀₋₁₇) and long-chain
452 (C₁₇₊) *n*-alkanes, yet they have different dominant carbon numbers, particularly C₁₉ for siltstones and
453 C₁₃ for the third and fourth intervals. As shown in [Figure 12](#) samples from the siltstone-enriched
454 Chang 6 and interval-1 tend to lie close to the apex of long-chain components to form Population I,
455 whereas samples of the intervals-3 and -4 that contain less long-chain molecules can be grouped into
456 Population III. We can also learn from [Figure 11](#) that different intervals produce different amounts of
457 extract yields. For example, interval-3 has produced the highest amount of thermal extracts per gram
458 rock, followed by interval-4 and interval-5. Irrespective of siltstones that yield smallest weight of
459 extracts, intervals-1 and -2 also produce relatively less thermal extract than do their shale
460 counterparts (intervals 3, 4 and 5).

461 The T_{vap}-GC-derived isoprenoid biomarker parameters, especially the ratios of pristane and phytane
462 as well as their adjacent *n*-alkanes, have been widely used as molecular indices to assess depositional
463 environment and organic matter type (Brooks et al., 1969; Powell and McKirdy, 1973; Didyk, 1978;
464 Powell, 1988; Peters et al., 1999; Peters et al., 2005). The concentrations of pristane, phytane, *n*-C₁₇
465 and *n*-C₁₈ show identical distributive patterns against depth throughout the studied succession in the
466 Zhang 22 well ([Figure 13](#)). For example, they are almost completely absent in the intervals-1 and -2,
467 and have slightly higher values in interval-5. Eight siltstones from the Chang 6 and interval-1, however,
468 possess extraordinarily high concentrations of those four compounds. Similarly, relatively higher
469 concentrations could also be found for the samples from the third and fourth intervals with respect to
470 their shaly counterparts. Although the ratio of pristane over phytane (Pr/Ph) has been normally
471 interpreted as the redox condition indicator based on a model for the origin of these two isoprenoids
472 (Didyk, 1978; Sofer, 1984; Peters et al., 1995), some limitations should be carefully considered when

473 applying that ratio in the range of 0.8-3.0 without other corroborating data (Peters et al., 2005). No
474 identification of particular depositional environment would be evolved in this study, yet the gradual
475 elevation of Pr/Ph still could reflect an increasingly oxidizing environment with increasing maturity
476 effect (Figure 13). By considering pristane and phytane with their adjacent *n*-alkanes, the ratios of
477 Pr/*n*-C₁₇ and Ph/*n*-C₁₈ display a relative scatter in the lithologically heterogeneous interval-1
478 compared to an uniform distribution downward (Figure 13). Most of these ratios from interval-1 are
479 plotted within the region that indicates reducing conditions, while others are demonstrated to be
480 rather indicative of mixed anoxic, dysoxic redox environments than of a solely reducing or oxidizing
481 condition (Figure 14). This interpretation is also supported by the distribution pattern of pyrite that it
482 is abundant in the organic-rich section including the intervals 1 and 2 (Population II), and depleted in
483 the lower, organic-lean section (intervals 3, 4 and 5).

484 Concentrations of monoaromatic as well as di- and triaromatic compounds from thermal extracts are
485 quantified for further characterizing the thermal evolution of retained petroleum (Ishiwatari and
486 Fukushima, 1979; Radke et al., 1982; Radke et al., 1986; Radke, 1988). These, together, represent the
487 bulk quantity of the aromatics (Figure 13), and remain relatively constant throughout 1540-1610 m
488 depth succession without regarding to abnormal values of several siltstone samples. In
489 monoaromatics, the gross dialkyl compound is the most predominant constituent, followed by the
490 trialkyl compounds. The abundances of these two kinds of monoaromatic homologues are slightly
491 elevated in interval-3, while the monoalkyl compounds are depleted compared to their overlying
492 and underlying counterparts. Furthermore, diaromatics are found significantly dominating over
493 triaromatics, and monoaromatics as well. On the mg/g TOC basis, sudden changes in the aromatic
494 distribution pattern for all aromatic homologues are observed in siltstone samples as well as in
495 thermal extracts in interval-3. Triaromatic compounds should be selected as evaluation of maturity
496 parameters, as their more condensed rings are not clearly separated by the gas chromatographic
497 system applied, while mono- and diaromatics seem to be affected by evaporation losses (Radke et al.,
498 1982). In our case, except for some concentrations in siltstones triaromatics remain remarkably
499 constant throughout the entire succession, which argue for the uniform thermal evolution in the
500 Zhang 22 well in favor of the consistent distribution of T_{max} values.

501 **4.8. Compositional Mass Balance Calculation**

502 The mass balance model derived from geochemical measurements has been applied for many years
503 to obtain a quantitative understanding of petroleum generation and migration (Claypool and Reed,
504 1976; Jones, 1981; Burns and Salot, 1986; Cooles et al., 1986). In our case, all investigated samples
505 are in the oil window, and immature samples or at least approximately immature with no significant
506 petroleum generation should be involved to represent the initial condition for the Chang 7 shale.
507 Normally, the sample should have a T_{max} value lower than or approaching to 435 °C, and resembles
508 shales from Zhang 22 well having the same type of kerogen and organic composition. A sample
509 (G014952, Type-I kerogen) of Chang 7 shale from our previous study (Pan et al., 2016) is marginally
510 mature with a T_{max} of 438 °C and production index (PI = 0.07) less than 0.1 (Espitalie et al., 1977;

511 Tissot and Welte, 1980; Peters, 1986). The superscripts ^{ma} and ^{im} denote the present-day conditions
512 for geochemical measurements of mature and immature samples, and superscript ⁱⁿⁱ refers to the
513 initial conditions within the present-day mature samples (Figure 15).

514 The GC-derived concentrations for each compound of currently mature samples are usually
515 normalized to the current TOC content, i.e., mg/g TOC^{ma}. These data, however, need to be
516 renormalized to the initial TOC (i.e., mg/g TOCⁱⁿⁱ) of the sample before generation and migration take
517 place, in order to calculate the volumes of expelled hydrocarbons by subtracting them from
518 concentrations of currently immature sample (mg/g TOC^{im}). Therefore, the key issue for a valid mass
519 balance calculation is the restoration of currently mature total organic carbon (TOC^{ma}) to initial total
520 organic carbon (TOCⁱⁿⁱ) when the shale was immature. For this purpose, we cited a hydrogen index
521 parameter (HI) expressed in mg of hydrocarbons per gram of the initial TOC (mg/g TOCⁱⁿⁱ) from Pelet
522 (1985):

523 Equation 1: $HI^{ini} = HI^{ma} \times (1200 - HI^{im}) / (1200 - HI^{ma})$,

524 where HI^{ma} = hydrogen index of mature sample as measured, and HI^{im} = measured hydrogen index of
525 immature sample; 1200 represents 1000 times of the reciprocal of 0.83, the assumed proportion of
526 carbon in Rock-Eval pyrolysis products. Therefore, for any given mature sample with measured TOC^{ma}
527 and HI^{ma} as well as HI^{im} for a selective immature sample from Rock-Eval pyrolysis, the initial TOC can
528 be expressed by:

529 Equation 2: $TOC^{ini} = TOC^{ma} \times (1200 - HI^{ma}) / (1200 - HI^{im})$.

530 With this knowledge, by applying the compositional mass balance model (Horsfield et al., 2001;
531 Santamara-Orozco and Horsfield, 2003), the original hydrocarbon generative potential of individual
532 component (C^{im} , mg/g TOC^{im}) for the selective immature sample, as well as the residual hydrocarbon
533 generative concentration of individual components normalized to the initial TOC (C^{ini} , mg/g TOCⁱⁿⁱ) for
534 each mature sample from the Zhang 22 well were calculated from Py-GC data. No renormalization for
535 the immature sample G014952 would be necessary because its concentration C^{im} expressed in
536 currently measured TOC^{im} represents the immature onset with which all other mature samples are
537 compared. Thus the generated concentration of individual component for each sample (C_g , mg/g
538 TOCⁱⁿⁱ) during natural subsurface maturation has been determined by subtracting the residual
539 generative concentration (C^{ini}) from the original potential (C^{im}) by:

540 Equation 3: $C_g = C^{im} - C^{ini}$.

541 The absence of such renormalization of individual components for the mature sample to its initial TOC
542 would cause an underestimation for the total hydrocarbon yield.

543 The results of the compositional mass balance calculation based on the aforementioned algebraic
544 scheme are further expressed in mg generated hydrocarbon per gram of rock. The average generated
545 *n*-alkane concentrations for each interval excluding gas fraction (C_{1-2}) are shown in Figure 16. The

546 generated hydrocarbons are compositionally dominated by light-end components with the highest
547 compound-specific concentration of n -C₄. The n -alkane concentrations remain constant with
548 increasing molecular weight until n -C₁₃ where they gradually decrease to zero approaching n -C₃₃. The
549 calculated generated amounts of hydrocarbons from eight siltstones as expected are extremely low
550 because they likely represents a reservoir in nature rather than a source rock. Intervals-3 and -4
551 produce more hydrocarbons compared to the siltstone samples, but still less productive than the
552 most organic-rich shale package (intervals-1, -2 and -5) whose samples have been classified into
553 Population II. Figure 12 shows three distinctive populations in which each group has different
554 composition with respect to relative content of chain length components. Samples from Chang 6
555 interval enriched the highest content of long chain length hydrocarbons over 17 carbon numbers are
556 typically extracted from tight reservoir, and are classified into Population I. These extracts were
557 retained in the layers closely adjacent to source rock in which fluids were charged and expelled
558 therein only leaving heavy-end moieties behind. Population II contains samples from the majority of
559 intervals-1, 2 and 5, and is principally composed by short-chain n -alkanes with carbon numbers
560 ranging from 1 to 10, in contrast to Population III that contains more longer moieties and is
561 dominated by samples from intervals-3 and 4. Population classification shows clear grouping patterns
562 for tight-oil-like Chang 6 interval, as well as the intervals-1, 2, 5 and intervals-3, 4 which will be
563 assigned as “generative units” and “in-source reservoir”, respectively, in the following discussion.

564

565 **5. Discussion**

566 **5.1. Oil retention within the stratified source rock**

567 The investigated Chang 7 succession of the Zhang 22 well can be subdivided into five intervals. Similar
568 to the sandy Chang 6 Member which has been assigned as a good reservoir, eight thin layers of
569 siltstone in interval-1 could be defined as ultra-tight reservoirs owing to the lean organic matter and
570 low pyrolyzable hydrocarbon yields (S_2). These samples also have high values of S_1 which represent
571 the quantity of hydrocarbons (oil + gas) currently preserved in the rock (Espitalie et al., 1977), as well
572 as the oil saturation index ($OSI = S_1/TOC \times 100$) greater than 100 mg/g TOC that has been
573 acknowledged as an indicator for potential producibility of oils (Lopatin et al., 2003; Jarvie, 2012).
574 Additionally, these findings are also supported by extract yields (> 200 mg/g TOC) that normalize the
575 weight of extracted hydrocarbons to total organic carbon (Figure 3). This phenomenon is not
576 surprising because all the above features are consistent with the properties of a petroleum reservoir
577 (Yang et al., 2015; Zou et al., 2015a; Xu et al., 2018).

578 Interestingly, there is a package of shales having the similar geochemical behavior as the siltstones,
579 essentially sourcing and reservoiring oil in the source rock. Interval-3 consists of black, organic-
580 containing (av. TOC = 3.56 wt%) shales with laminated beddings composed of a mix of flakes of clay
581 minerals and tiny fragments (silt-sized particles) of other minerals (Figure 5-i and j). These shales are
582 mineralogically dominated by clays (Table 2), and pyrite is absent. They have average S_2 yields of 6.91

583 and 3.16 mg HC/g rock before and after the Soxhlet extraction, respectively, which gives the quantity
584 of hydrocarbons that the rock could still produce should burial and maturation continue (Espitalie et
585 al., 1977). Interval-3, undoubtedly, could be defined as a source rock.

586 Nevertheless, an obvious T_{max} values decline occurs in interval-3 (Figure 3), compared to values seen
587 in the shales from other intervals which display a constant T_{max} profile. The eight siltstones have
588 extremely low values of T_{max} because they are not source rocks. This low T_{max} level for interval-3
589 could be ascribed to the presence of involatile, heavy bitumen (Kruger, 1983). For example, the T_{max}
590 values (av. $T_{max} = 436^{\circ}\text{C}$ [816 $^{\circ}\text{F}$]) have shifted to a higher level (av. $T_{max} = 461^{\circ}\text{C}$ [861 $^{\circ}\text{F}$]) after Soxhlet
591 extraction (Figure 17 and Table 3). This T_{max} shift phenomenon has also been reported for the Barnett
592 Shale (Han et al., 2015). In addition, notably high yields of S_1 (Table 3) and relatively low contents of
593 TOC result in OSI values that are greater than 100 mg/g TOC, indicating an oil crossover effect that
594 denotes potentially producible oils (Pepper, 1991; Sandvik et al., 1992; Jarvie et al., 1996; Jarvie,
595 2012). This empirical OSI value, however, does not rule out the possibility of producible oils for those
596 having an OSI less than 100 mg/g TOC, because the measured S_1 values are often underestimated due
597 to the loss of light oil during sample handling and preparation (Jarvie and Baker, 1984; Cooles et al.,
598 1986). The yields of extractable hydrocarbons exceed more than 200 mg/g TOC in interval-3, which
599 strongly supports this crossover effect (Figure 3). Furthermore, the remarkable elevation of HI values
600 in interval-3 also reflects the contribution of an involatile fraction from the retained petroleum or
601 bitumen to the S_2 peak (Han et al., 2015). HI values are significantly reduced after the retained oil has
602 been extracted (Figure 17). Therefore, oil retention occurs in interval-3 which can be defined as an in-
603 source reservoir (i.e., reservoir interbedded in the source rock or oil saturated sweet spots in the
604 source rock). In short, this interval is a stratigraphic succession with geochemical features consistent
605 with those of a source rock but containing retained oil or bitumen like a normal reservoir does.

606 Rock-Eval pyrolyses before and after extraction were used to examine oil retention phenomena in the
607 Zhang 22 well. (Figure 18 and Table 3). After extraction, free hydrocarbons in the rock (S_1) were
608 essentially eliminated (Figure 17), and the S_2 peak reduced in intensity as the involatile fraction of
609 retained oil was eliminated (Figure 17). Siltstones and shales from interval-3 are characterized by the
610 extensive reduction of S_2 value after extraction because the highest proportion of retained oil is
611 presented in such so-called reservoir or in-source reservoir (Figure 18-a and d). Note that there are
612 pre-shoulders ahead of S_2 peaks which indicate that by adsorbing on rock matrix, the heavy molecular
613 weight compounds of retained oil were subjected to cracking during pyrolysis before the main stage
614 of thermal degradation of kerogen (Barker, 1974; Clementz, 1979; Dembicki et al., 1983). The minor
615 pre-shoulder is also presented in interval-4 (Figure 18-e). These “pre-shoulders” are successively
616 removed after the retained hydrocarbons have been solvent-extracted. In addition, T_{max} shifts could
617 be found in the pyrograms (Figure 18-a and d). Minor change of T_{max} also appears in interval-4 (Figure
618 18-e).

619 Although the pyrolytic character of shales from interval-4 are quite similar to those from the overlying
620 interval-3 due to the presence of bitumen, more detailed geochemical or molecular information is

621 needed to safely classify interval-4 as an in-source reservoir. The bulk geochemistry of extracts shows
622 that intervals-3 and -4 have similar fractional composition (Figure 10): aliphatic hydrocarbons account
623 for more than three quarters of total extractable components, compared to the counterparts from
624 the intervals 1, 2 and 5 which contain less saturated hydrocarbons, but more polar and aromatic
625 compounds. This chemical composition appears in the reservoir samples – the siltstones – as well.
626 Higher proportions of aliphatic hydrocarbons (81% for interval-3 and 76% for interval-4) versus
627 aromatic compounds and resins in the total extracts are ascribed to the preferential retention of oil
628 during generation and expulsion in the order of polar compounds (resins) > aromatic hydrocarbons >
629 aliphatic hydrocarbons (Leythaeuser et al., 1988; Sandvik et al., 1992). Additionally, intervals-3 and -4
630 tend to be dominated by intermediate-chain to long-chain *n*-alkanes, which resemble most closely
631 those extracted from siltstones; their counterparts, intervals-1, -2 and -5, clearly possess a higher
632 proportion of lighter homologues in the total saturated hydrocarbons from thermovaporization
633 (Figure 12). These trends might result from the chromatography-like fractionation effects according to
634 polarity during primary migration and expulsion (Leythaeuser et al., 1984), which will be discussed
635 later. Thus, we consequently refer intervals-3 and -4 as “in-source reservoirs” (sweet spots) in which
636 more oils tend to be retained and preserved than in other intervals.

637 In contrast, shales from intervals-1, -2 and -5 show no obvious pre-shoulder phenomenon and T_{max}
638 shift (Figure 18-b, c and f). Their bulk geochemistry and the compositional distribution of extracts
639 resemble each other yet differ from those having a high residual bitumen content. These three
640 intervals, therefore, are the main “generative units” in the Zhang 22 well. Owing to this difference
641 between reservoir unit and generative unit in the nature, sudden changes in the aromatic distribution
642 pattern for all aromatic homologues in the intervals-3 and -4 on the mg/g TOC basis (Figure 13) can be
643 attributed to the oil retention effects that make abundances per gram TOC overestimated. Meanwhile,
644 concentrations of pristane and phytane are much lower than those of closely eluting *n*-alkanes (*n*-C₁₇
645 and *n*-C₁₈) in the in-source reservoir (Figure 13) because isoprenoids are expelled less effectively than
646 the adjacent *n*-alkanes (Leythaeuser et al., 1984).

647 5.2. Quantification of Retained Hydrocarbons

648 The total volatizable yield (S_1) and the amount of total soluble extract (TSE) have been widely used in
649 determining the amount of retained petroleum (Claypool and Reed, 1976; Espitalie et al., 1977;
650 Cooles et al., 1986; Peters, 1986), yet merely using S_1 values to represent the total oil content would
651 lead to an underestimation because of absorption to the rock matrix. Heavy moieties (C₁₇₊) of
652 retained oil may be thermally carried over into the S_2 peak (i.e., the pre-shoulders in Figure 18)
653 (Barker, 1974; Dembicki et al., 1983; Han et al., 2015). Thermal solvent-extraction, on the other hand,
654 would not retain light hydrocarbons (C₅₋) during solvent evaporation (Jarvie and Baker, 1984) but
655 could effectively draw out the heavy-end fractions that are neglected by the Rock-Eval approach. In
656 this study, thermal solvent-extraction yields excellently correlate with Rock-Eval S_1 values, but are
657 almost twice the size of S_1 values (Figure 19-a). Thus, we hereby apply a quantitative calculation from
658 Han et al. (2015) who made a modification from the original equation proposed by (Jarvie, 2012):

659 Equation 4: Total oil content = $S_1^{\text{wholerock}} + (S_2^{\text{wholerock}} - S_2^{\text{extracted rock}})$,

660 and the results are shown in [Figure 19-b](#) and [Table 3](#). Even though calculated total oil contents are the
661 minimum values, they display a good correlation with S_1 and extract yields (for both $R^2 = 0.99$). They
662 are 1.95 times higher than S_1 values, but are approximately equal to extract yields ([Figure 19-b](#)).
663 Concerning the average total oil content throughout the shale, interval-3 and -4 as expected, are the
664 most prolific targets with in-place resource potential twice that of the organic-rich counterparts
665 interval-1, -2 and -5 ([Table 3](#)). Interestingly, the organic-rich reference dataset of Chang 7-3 also
666 shows a comparably high amount of retained oil or bitumen (8.77 mg/g rock) which could have been
667 preserved or formed during deposition and diagenesis of the Chang 7 shale.

668 5.3. Hydrocarbon Expulsion Efficiency

669 By calculating the average concentration of individual n -alkanes of the retained oil for each interval
670 from the T_{vap}-GC data ([Figure 16-right column](#)), the compositional amount of expelled hydrocarbons
671 can consequently be quantified by subtracting retained n -alkanes from the formerly calculated
672 generation yields from pyrolysis ([Figure 16-left column](#)):

673 Equation 5: $C^{\text{expelled}} = C^{\text{generated}} - C^{\text{retained}}$.

674 Furthermore, the compositional expulsion efficiency (%) for each interval, therefore, can be
675 represented by the ratio of the average concentration of expelled hydrocarbons over the average
676 concentration of generated hydrocarbons:

677 Equation 6: $E^{\text{expulsion}} = C^{\text{expelled}} / C^{\text{generated}} \times 100$.

678 [Figure 20](#) gives the results of each interval's average expulsion concentration and efficiency for
679 individual n -alkanes. The residual light-end n -alkanes ($< C_{13}$) from the evaporative losses of light
680 moieties, presumably being more mobile (Mackenzie et al., 1983), were expelled more efficiently than
681 the heavy-end during primary migration with the highest expulsion concentration and efficiency at n -
682 C_4 . The expelled concentrations gradually decrease with increasing molecular weight, and approach
683 zero at n - C_{33} ([Figure 20-left column](#)). In siltstones and the formerly defined in-source reservoirs
684 (intervals-3 and -4), negative value of expulsion concentrations appear among intermediate- to long-
685 chain length range (normally from C_{13} to C_{25}), indicating that more hydrocarbons are stored in place
686 than could have been generated from kerogens within the particular interval, and additional
687 hydrocarbons must have been migrated from other layers and been accumulated therein. More
688 specifically, more light molecular weight hydrocarbons tend to be retained in interval-3 compared to
689 siltstone layer and the underlying interval-4 with the highest concentration of individual n -alkane at n -
690 C_{17} ([Figure 20](#)). Thus, the expulsion calculation support our aforementioned classification to define
691 interval-4 having oil retention effects, even though its quantity is much lower than the main retained
692 interval-3. For the generative units in the Zhang 22 well (intervals-1, -2 and -5), no negative value of
693 expulsion concentration can be observed, and the gradual decrease of concentrations along with

694 lengthening *n*-alkane chains favor the claims that no significant expulsion is suspected beyond *n*-C₂₅
695 (Mackenzie et al., 1983; Leythaeuser et al., 1984).

696 The calculated expulsion efficiencies show an initial decrease and then increase trend as carbon
697 number increases (Figure 20-right column). The highest expulsion efficiencies of around 98% are
698 observed for *n*-alkanes up to *n*-C₆ except for interval-2 in which the expulsion efficiency decreases
699 significantly to 84.54% at *n*-C₆, whereas the lowest values are commonly found in different chain
700 length ranges much more pertinent to the retained or generative nature for each interval. For
701 example, the in-source reservoirs (siltstone, intervals-3 and -4) reach the negative value of expulsion
702 efficiency at very long-chain length range near to *n*-C₂₀ similar to the concentration distribution of
703 expelled hydrocarbons; the generative intervals in nature (intervals-1 and -2), however, approach the
704 lowest positive efficiency in short-chain length range (near *n*-C₁₀), and tend to expel more
705 intermediate- to long-chain hydrocarbons efficiently. Afterward as chain length increases, the
706 calculated expulsion efficiencies rise up again reaching up to 98% at *n*-C₃₂. This is unaccepted because
707 heavy molecular weight compounds should be less mobile and preferentially retained (Mackenzie et
708 al., 1983; Ritter, 2003). This is, therefore, probably an artificial error caused by the limitation of T_{vap}-
709 GC approach, in which long-chain length compounds (normally > C₁₇) tend to be subjected to
710 incomplete thermal evaporation because the T_{vap}-GC technique is usually performed isothermally at
711 300 °C (Han et al., 2015). This limitation brings about an underestimation of the retained
712 concentration of heavy-end compounds. Thus, the expulsion efficiencies would be overestimated
713 along with increasingly higher molecular weight.

714 In order to readily compare the intervals with one another, mass balance profiling was undertaken
715 using a single selected compound (*n*-C₁₇) (Figure 21). Clearly, most samples from intervals-1, -2 and -5
716 generate larger quantity of *n*-C₁₇ hydrocarbons than do intervals-3 and -4. By contrast, samples from
717 the intervals-3 and -4 retain more *n*-C₁₇ than they could have been generated at present maturity.
718 Pertinent to the generated and retained distribution of *n*-C₁₇, expulsion amounts of *n*-C₁₇ are negative
719 in intervals-3 and -4 as well as eight siltstone samples indicating oil retention effects compared to
720 those positive values observed in the intervals-1, -2 and -5. In addition, the expulsion efficiency shows
721 the same distributive trend of *n*-C₁₇ as the above parameters do. It is clear that the intervals-3 and -4
722 can be safely referred to as “in-source reservoirs” in the studied Chang 7 shale, at least in the Chang
723 7-1 and Chang 7-2 units, which are more likely sourced by the overlying organic-rich shales.

724 **5.4. Controls on Hydrocarbon Storage in Shales**

725 Many authors have investigated the various controlling factors on petroleum retention in source
726 rocks. For example, Pepper (1991) proposed that kerogen composition plays an important role in
727 determining expulsion efficiency. Sandvik et al. (1992) argued that the selective absorption of
728 generated petroleum within solid organic matter is a significant phenomenon and is one cause of
729 compositional differences between migrated liquids and retained bitumen in the source rock. Jarvie
730 et al. (2007) have further reviewed the gas storage capacity in organic-rich shale by studying gas or oil

731 chemically adsorbed to or physically absorbed within the organic matrix, and concluded that organic
732 richness, kerogen type, and thermal maturity impact the sorptive capacity of organic matter. Despite
733 the above organic matter properties, inorganic characteristics, such as mineralogical composition,
734 porosity, permeability, fractures and cementation, also exert substantial control upon hydrocarbon
735 retention (Han et al., 2015). For example, some minerals, such as illite and montmorillonite, have
736 remarkable BET surface area (26 m²/g for pure illite and 30 m²/g for pure montmorillonite) and thus,
737 are capable of sorbing gas in their internal structure (Schettler and Parmely, 1991; Ross and Marc
738 Bustin, 2009). Consequently, total porosities in clay-rich shales are larger than those in silica-rich
739 shales due to open porosity associated with the aluminosilicate fraction (Ross and Marc Bustin, 2009).

740 For our case study, the relationship between Rock-Eval S₁ and TOC content (Figure 22-a) illustrates
741 that organic richness substantially controls hydrocarbon retention effect in the studied sample set.
742 Organic abundance seems to exert much stronger influence upon the petroleum retention in the in-
743 source reservoirs (intervals-3 and -4) than in generative units (intervals-1, -2 and -5), even though
744 both units have retentive capacity positively correlated with TOC content. It is obvious that with the
745 increasing quartz content the retained amount in the oil saturated sweet spots significantly increases,
746 but that in the generative units decreases accordingly (Figure 22-b). Nevertheless, these positive and
747 negative relationships between quartz and retention abundance are restricted to a narrow range
748 (10% < quartz < 30%), because of the smaller amounts of petroleum being associated with storage in
749 quartz compared to illite and kerogen (Schettler and Parmely, 1991). The greater the quartz content
750 in the mineralogical composition, the less clay minerals present, and consequently the less petroleum
751 volume that is retained in the shale.

752 Following the approach of Han et al. (2015), we present two formulae using binary linear regressions
753 for quantitatively describing the contributions of TOC and quartz contents to hydrocarbon retention:

754 Equation 7: $S_1^{cal} = 0.131 \times \text{TOC} + 0.163 \times \text{Quartz} - 0.475$ (for in-source reservoirs)

755 Equation 8: $S_1^{cal} = 0.110 \times \text{TOC} - 0.009 \times \text{Quartz} + 1.390$ (for generative units)

756 After calculation of the retained amount of petroleum (S₁^{cal}) considering the contribution of organic
757 abundance (TOC) and quartz content, a modest overall correlation (R² = 0.642) between calculated S₁
758 and measured S₁ values was observed in Figure 22-c. Organic richness has the same weighting as
759 quartz for retention effects in the in-source reservoirs (coefficients 0.131 over 0.163), whereas in the
760 generative units its influence is much stronger (0.110 versus 0.009). Moreover, quartz content
761 imposes more influence on hydrocarbon storage in the in-source reservoirs than in the generative
762 units (coefficients 0.163 versus -0.009) which is comparable to the data for the relationship between
763 S₁ values and quartz content (Figure 22-b) wherein quartz in the generative units shows a negative
764 correlation with increasing S₁ values.

765 If the TOC is replaced by pyrolyzable hydrocarbons (S₂) for calculating the retained S₁ the role of live
766 carbon for sorption and retention can be assessed (Han et al., 2015; Mahlstedt and Horsfield, 2015):

767 Equation 9: $S_1^{cal'} = 0.197 \times S_2 + 0.150 \times \text{Quartz} - 1.097$ (for in-source reservoirs)
768 Equation 10: $S_1^{cal'} = 0.066 \times S_2 - 0.012 \times \text{Quartz} + 1.591$ (for generative units)

769 Although the coefficient determination ($R^2 = 0.672$) between $S_1^{cal'}$ and measured S_1 is only slightly
770 raised in Figure 22-d compared to that in a S_1^{cal} and measured S_1 determined linear regression ($R^2 =$
771 0.642 in Figure 22-c), the “live” or labile carbon indicated by S_2 value has been reported a
772 contribution to sorptive capacity in the kerogen (Han et al., 2015). Nonetheless, when inert kerogen is
773 excluded from the calculation, the thermally labile carbons are more important in sorbing
774 hydrocarbons onto their surface for the in-source reservoirs (coefficients 0.197) than for the
775 generative units (coefficients 0.066). The organic factors (e.g., S_2) predominantly exert influence on
776 both units, and the inorganic one (quartz) still plays more important role on the in-source reservoirs
777 than the generative ones, no matter whether replacing the total organic richness by labile carbons.

778 5.5. Intrasource Fractionation and Migration

779 By comparing the geochemical and molecular composition of samples from the organic-leaner in-
780 source units and from the organic-rich generative intervals, the stored petroleum in intervals-3 and -4
781 consists of more aliphatic hydrocarbons, whereas that in intervals-1, -2 and -5 is more aromatic and
782 polar (Figure 10 and Table 4). In association with the mass balance calculations for each interval, the
783 high expulsion efficiencies of the organic-rich generative units, particularly interval-2 and 5, would
784 initiate a preferential intraformational migration of aliphatic hydrocarbons into the adjacent relatively
785 organic-leaner in-source reservoir units, i.e. intervals-3 and -4, which are characterized by low, even
786 negative value of expulsion efficiencies (Figures 20 and 21). Although this observation is parallel to
787 the experimental data which have proposed a preferential migration order as *aliphatic*
788 *hydrocarbons > aromatic hydrocarbons > polar compounds* (Leythaeuser et al., 1988; Sandvik et al.,
789 1992; Han et al., 2015), low proportions of aromatic and polar compounds in the in-source reservoirs
790 were observed and might result from a compositional dilution of these less mobile compounds by
791 migrated aliphatic hydrocarbons and thus, leave behind more of these retainable compounds in the
792 generative units, e.g. interval-2 and 5. In addition, the different generation and expulsion capabilities
793 of interval-2 and 5 result from different organic richness, and consequently bring about more
794 petroleum being retained in interval-3 than being in interval-4.

795 Moreover, *n*-alkanes can be subjected to molecular fractionation during intrasource migration
796 (Mackenzie et al., 1983), that is, for our case study, heavy-end *n*-alkanes being found preferentially
797 retained in the third and fourth interval (in-source reservoirs), while light-end compounds are
798 enriched in intervals-1, -2 and -5 (generative units) (Figures 11 and 12). Commonly, light-end
799 hydrocarbons are believed to be preferentially migrated; however, if the migration direction is
800 presumably from intervals-1, -2 and -5 to intervals-3 and -4, they are still found to be enriched in
801 generative units rather than in the in-source reservoirs (Figure 11). The migration effect of generated
802 hydrocarbons are explainable by many possible models of primary migration (Tissot et al., 1971), yet a
803 pressure-driven, hydrocarbon phase movement should be considered as the dominating primary

804 migration mechanism for the Chang 7 shale in the Zhang 22 well, due to the lack of available
805 information for other possibilities, such as microfractures caused by pressure build-up. Based on this
806 assumption, high organic content intervals (e.g. interval-2) would generate hydrocarbons earlier and
807 greater than their leaner counterparts (e.g. interval-3), in which increasingly elevated bitumen
808 concentration in the generative units during source rock maturation would act as the driving force for
809 fluid movement from generative units to in-source reservoirs alongside decreasing pressure gradient.
810 Consequently, light-end *n*-alkanes are enriched in the generative units compared to that in the in-
811 source reservoirs. Furthermore, only nonefficient expulsion of generated and migrated petroleum
812 would cause an enrichment of light-end *n*-alkanes in interval-3 or -4. The expulsion efficiencies for
813 individual hydrocarbon in the in-source reservoirs, however, are clearly very high for carbon numbers
814 reaching up to *n*-C₈ compared to those in adjacent generative units (Figure 20). For example, the
815 expulsion efficiencies for heptane in intervals-3 and -4 (84.61% and 86.77%, respectively) are
816 significantly higher than those of intervals-2 and -5 (74.68% and 77.29%, respectively). Retention of
817 additional liquid petroleum only occurs for the carbon numbers higher than *n*-C₁₀ in interval-3 and
818 C₁₄ in interval-4. Therefore, the higher expulsion efficiency of light-end hydrocarbons in the in-source
819 reservoirs than that in the generative units makes these light *n*-alkanes easily depleted, showing a
820 relative low concentration of light end moieties in the in-source reservoirs. Hydrocarbon depletion
821 during sample handling could be another possibility for the lack of shorter *n*-alkanes in intervals-3 and
822 -4, which is due to the relative higher porosity and easier to lose those compounds after samples
823 were exposed to the air.

824 6. Conclusions and Significance

825 The studied mature Chang 7-1 and Chang 7-2 units in the Zhang 22 well consist of two types of
826 lithofacies, namely siltstone and shale. Oxidic, basinal environment-deposited siltstones contain a
827 higher proportion of terrigenous clastic minerals such as feldspar and allogenetic quartz, and lack
828 pyrite. They are organic-lean (av. TOC = 0.85 wt%) with lowest amount of pyrolyzable hydrocarbons
829 ($S_2 = 1.58$ mg HC/g rock). In contrast, the shales displayed a lack of distinctive cyclicality, and were
830 deposited under a continuous, stable reducing environment with no obvious sign of subaerial
831 exposure or evaporite formation. These sediments contain more than 40% clay minerals and average
832 3% pyrite. These organic-rich black shales are characterized by an average TOC value greater than
833 5.86% and more pyrolyzable hydrocarbons (av. $S_2 = 8.45$ mg HC/g rock) than those of the siltstones.
834 The Chang 7 shale is the most prolific source rock in the Yanchang petroliferous system, and can be
835 subdivided into five intervals based on the mineralogical and geochemical composition.

836 The Chang 6 consists of siliceous siltstones and is a typical tight reservoir in contact with adjacent
837 organic-rich source rocks, which is characterized by the lowest organic content (av. TOC = 0.85 wt%)
838 and S_2 values but by the highest free oil contents and OSI values compared to the Chang 7 shale.
839 Unlike the other four intervals that are homogeneously composed of shales, interval-1 lithologically
840 consists of six siltstones and twenty four shales (mudstones). It contains high TOC content (5.98 wt%)
841 and preserves high hydrocarbon generative potential ($S_2 = 8.07$ mg HC/g rock). The second interval

842 represents the best source in the Chang 7 shale with the highest organic matter content (av. TOC =
843 8.73 wt%) and average S_2 value (12.77 mg HC/g rock). These two intervals have been defined as the
844 “generative units” in the Chang 7 shale. In contrast, the leanest interval, interval-3, contains the
845 highest free oil content determined by the pyrolysis approach (av. S_1 = 3.62 mgHC /g rock) and
846 extractable yields (8.94 mg HC/g rock and 256.66 mg HC/g TOC), having oil crossover effect (OSI > 100
847 mg HC/g TOC), T_{max} shift phenomenon, as well as the HI being shifted to higher values. Although the
848 fourth interval shows no obvious crossover effect and shift phenomenon, its solvent extracts have
849 similar chemical compositions to those of interval-3, and contains more aliphatic hydrocarbons than
850 the generative units, interval-1 and interval-2, as well as the Chang 6 siltstones. It also contains more
851 heavy-end *n*-alkanes which is similar to interval-3. Thus, interval-3 and interval-4 are described as “in-
852 source reservoir units” or “sweet spots”. The fifth interval is leaner than intervals-1 and -2, but still
853 resembles the features that a generative unit should have.

854 Geochemical and molecular compositions display distinctive differences between stored oils from the
855 generative units and from the in-source reservoirs. Bitumens from the generative units (intervals-1, -2
856 and -5) have the proportional composition of saturated hydrocarbons from 56% to 66%, significantly
857 lower than that from the in-source reservoirs (interval-3, 4 and Chang 6 siltstone), which contain an
858 aliphatic fraction up to 81%. Accordingly, the proportions of aromatic components and resins of the
859 generative units are higher than that of the in-source reservoirs. Besides, more light-end *n*-alkanes
860 are enriched in the generative units, compared to the more heavy-end moieties that are gathered in
861 the in-source reservoirs. Furthermore, the overall and the compound-specific expulsion efficiencies
862 for each interval calculated from the compositional mass balance support the differentiation scheme
863 for the Chang 7 shale. Samples having a generative nature show positive expulsion efficiency, whereas
864 those from the in-source reservoirs are accordingly negative. These negative values indicate that
865 more petroleum was present in the in-source reservoirs than could have been generated by the
866 kerogen during thermal maturation, i.e., there are extra hydrocarbons that have accumulated in these
867 reservoir units.

868 On estimating the amounts of expelled and retained hydrocarbons in the Chang 7 shale system we
869 realize that the amount of oil-in-place was systematically underestimated by 51.28% if we merely take
870 unextracted S_1 values into consideration, because heavy-end hydrocarbons (C_{17+}) would be thermally
871 carried over into the S_2 peak. Similarly, the remaining generation potential would also be
872 overestimated if the extraction and correction are not considered. In addition, the oil retention effect
873 will bring about T_{max} shifting to lower values, returning to the “normal” levels after extracting the free
874 oil in the rocks. This can also be ascribed to the carryover of S_1 heavy molecular weight compounds
875 into the S_2 temperature range before the main stage of thermal degradation of kerogen. An amended
876 assessment of total amount of oil-in-place, therefore, has been introduced into this study to
877 overcome the aforementioned misestimations when quantifying the retained petroleum in the Chang
878 7 shale system.

879 The enrichment of aliphatic compounds in extracts from the in-source reservoirs versus the
880 enrichment of aromatic and polar hydrocarbons in those from the generative units can be ascribed to
881 the differential retention of compounds during primary migration. Specifically, the polar compounds
882 tend to be retained in place and aliphatic hydrocarbons are preferentially migrated from generative
883 units to the in-source reservoirs, while the aromatic hydrocarbons have mobility between these two
884 compounds. In addition, preferential expulsion of light molecular weight compounds also occurs
885 compared to heavier molecular weight compounds during primary migration. Therefore, a vertical
886 migration pathway or a model could be speculated that the generated liquids are expelled into
887 interval-3 and interval-4 from the overlying units (interval-1 and interval-2) and the underlying
888 interval-5. These findings coincide with the negative value of expulsion efficiencies of the in-source
889 reservoirs, which indicate extra liquids have accumulated in these intervals with respect to their
890 generative capabilities.

891 The stored petroleum within the generative units is primarily controlled by organic matter richness,
892 especially the “labile” component (S_2) rather than the TOC alone. However, the retained oils in such
893 in-source reservoirs are seemingly not only controlled by organic richness, but also by having positive
894 relationship with quartz content. The secondary matrix porosity in interval-3 and interval-4 would
895 play a critical role for storing more oil in the in-source reservoirs than in the generative units.

896 The most significance for the local petroleum industry is that the in-source reservoirs in the Chang 7
897 shale, i.e. interval-3 plus interval-4, can be the most promising target or sweet spot for shale oil
898 exploration and production. The retained oils have been migrated and expelled within source rock
899 system through geological time, and the stratigraphic fractionation makes oil quality improved
900 containing more aliphatic fraction. This geochemical composition likely makes oils having higher
901 removability in the in-source sweet spot. Furthermore, the extra storage potential of shale, as well as
902 the weak adsorptive affinity of oil to organic matter collectively account for a good productive
903 potential of shale oil. Additionally, in conjunction with the high degree of brittleness, low content of
904 TOC, and taking shale frackability into consideration, the in-source reservoirs are a set of attractive
905 sweet spots (i.e., intervals-3 and -4) for hydrocarbon production in the Chang 7 shale system of the
906 Ordos Basin.

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1177 **Figure captions:**

1178 **Figure 1.** Sketch map showing (a) location of Ordos Basin in China mainland; (b) tectonic units, shale
 1179 thickness distribution and study area; as well as (c) an east-west cross section. Age symbols
 1180 descriptions: Pt₂₊₃ = Middle *plus* Upper Proterozoic; C = Cambrian; O = Ordovician; C = Carboniferous;
 1181 P = Permian; T = Triassic; J = Jurassic; K = Cretaceous; E = Paleogene; N = Neogene; Q = Quaternary; Pz
 1182 = Paleozoic; Mz = Mesozoic. The shale thickness refers to Zou (2013).

1183 **Figure 2.** Stratigraphic columns, depositional environment and source-reservoir-seal associations from
 1184 Upper Triassic to Quaternary in the Ordos Basin.

1185 **Figure 3.** Mineral composition (pyrite, quartz, feldspar and clay), Rock-Eval derived S₁, S₂ and T_{max}
 1186 (including HI, OI and OSI), as well as rock sample extract yields *versus* depth profile of the Zhang 22
 1187 well in the Ordos Basin showing geochemical and mineralogical compositions, and subdivision of
 1188 studied succession. GR = Gamma Ray logging; S₁ = amount of thermally extractable hydrocarbons
 1189 volatilized at 300 °C (572 °F, mg HC/g rock); S₂ = amount of hydrocarbons generated by pyrolysis
 1190 between 300 and 650 °C (572 °F and 1202 °F, mg HC/g rock); TOC = Total Organic Carbon (wt.%); OSI =
 1191 Oil Saturation Index (S₁/TOC×100, mg HC/g TOC); HI = hydrogen index (S₂/TOC×100, mg HC/g TOC); OI
 1192 = oxygen index (S₃/TOC×100, mg CO₂/g TOC); T_{max} = temperature at which the rate of S₂ generation is
 1193 at maximum (°C); Extract yield = amount of extractable hydrocarbons in Soxhlet extraction using
 1194 azeotropic solvent system for 24 h at 60 °C (140 °F) (mg HC/g TOC or mg HC/g rock). Chang 7-3 data
 1195 points are from Pan et al. (2016).

1196 **Figure 4.** Ternary diagram of the bulk mineralogical composition showing relative concentration of
 1197 clay minerals, carbonate and quartz. Two lithofacies can be distinguished as argillaceous and siliceous
 1198 lithofacies denoted by solid line and stippled line, respectively.

1199 **Figure 5.** Photomicrographs showing lithological compositions. **(a)** G016048, siltstone from Chang 6,
 1200 depth 1539.19 m (5049.84 ft), parallel to bedding, under cross-polarized light; siltstone containing
 1201 quartz and feldspar. **(b)** G016049, shale from interval-1, depth 1540.09 m (5052.78 ft), perpendicular
 1202 to bedding, under polarized light; laminated shale containing lamalginite and quartz. **(c)** G016049,
 1203 shale from interval-1, depth 1540.09 m (5052.78 ft), parallel to bedding, under reflected white light;
 1204 pyrite framboids. **(d)** G016066, siltstone from interval-1, depth 1555.35 m (5102.85 ft), parallel to

1205 bedding, under cross-polarized light; shale containing quartz and feldspar minerals. **(e)** G016079,
1206 shale from interval-2, depth 1567.01 m (5141.11 ft), perpendicular to bedding, under polarized light;
1207 laminated shale with lamalginite in the quartz and feldspar matrix. **(f)** G016079, shale from interval-2,
1208 depth 1567.01 m (5141.11 ft), parallel to bedding, under fluorescent light (blue light excitation) in oil
1209 immersion; alginite particle containing bitumen in the organic pore. **(g)** G016087, shale from interval-
1210 2, depth 1574.19 m (5164.66 ft), perpendicular to bedding, under fluorescent light (blue light
1211 excitation); alginite particle. **(h)** G016087, shale from interval-2, depth 1574.19 m (5164.66 ft), parallel
1212 to bedding, under reflected white light; pyrite framboids. **(i)** G016091, shale from interval-3, depth
1213 1577.78 m (5176.44 ft), perpendicular to bedding, under polarized light; homogeneous shale
1214 containing dispersed organic matter in the argillaceous matrix with quartz and feldspar. **(j)** G016091,
1215 shale from interval-3, depth 1577.78 m (5176.44 ft), parallel to bedding, under reflected white light;
1216 pyrite and terrigenous fusinite in the organic-rich shale. **(k)** G016100, shale from interval-4, depth
1217 1585.86 m (5202.95 ft), perpendicular to bedding, under reflected white light; pyrite framboids. **(l)**
1218 G016108, shale from interval-4, depth 1593.04 m (5226.50 ft), perpendicular to bedding, under
1219 polarized light; laminated shale with lamalginite and quartz. **(m)** G016115, shale from interval-5,
1220 depth 1599.32 m (5247.11 ft), parallel to bedding, under polarized light; homogeneous shale
1221 containing dispersed organic matter in the argillaceous matrix with quartz and feldspar. **(n)** G016115,
1222 shale from interval-5, depth 1599.32 m (5247.11 ft), parallel to bedding, under reflected white light;
1223 pyrite framboids. **(o)** G016115, shale from interval-5, depth 1599.32 m (5247.11 ft), parallel to
1224 bedding, under fluorescent light (blue light excitation); amorphous organic matter dispersed in the
1225 argillaceous matrix.

1226 **Figure 6.** S_2 yields plotted *versus* TOC content with lines of similar hydrogen index values. Modified
1227 from Langford and Blanc-Valleron (1990).

1228 **Figure 7.** Kerogen typing of the studied samples and reference dataset based on **(a)** pseudo van
1229 Krevelen diagram and **(b)** T_{max} *versus* hydrogen index diagram.

1230 **Figure 8.** Pyrolysis-GC-derived compounds in determining **(a)** kerogen typing according to the relative
1231 abundance of *n*-octene, (*meta* + *para*)-xylene and phenol (Larter, 1984a), and **(b)** molecular structure
1232 of kerogen based on *ortho*-xylene, *n*-nonene and 2,3-dimethylthiophene (Eglinton et al., 1990).

1233 **Figure 9.** Relationship between predicted petroleum type organofacies and chain length distribution
1234 determined by open-system pyrolysis gas chromatography (Py-GC). $C_1 - C_5$ = total resolved
1235 pyrolysates; $C_6 - C_{14}$ = sum of resolved *n*-alkenes and *n*-alkanes; C_{15+} = sum of resolved *n*-alkenes and
1236 *n*-alkanes. Modified from Horsfield (1989, 1997).

1237 **Figure 10.** Average chemical composition of extracts for each interval and overall succession. Note
1238 that “siltstones” represent those from the Chang 6 and the first interval, and no such sample is
1239 included when calculating the average value for the single interval-1.

1240 **Figure 11.** T_{vap}-GC-derived *n*-alkanes distributions of individual samples from each interval. Eight
1241 siltstones are combined from Chang 6 and the first interval to address the similar distributive pattern.
1242 The *x*-axis indicates carbon numbers of the chain length of *n*-alkanes.

1243 **Figure 12.** T_{vap}-GC-derived *n*-alkane distribution diagram showing the relative abundance of sums of
1244 n - C_{1-10} , n - C_{11-16} and n - C_{17+} .

1245 **Figure 13.** T_{vap}-GC-derived acyclic isoprenoids pristane, phytane and the ratio with their adjacent *n*-
1246 alkanes, as well as mono-, dia- and tri-aromatics *versus* depth profile. Siltstone samples are referred
1247 to as “s.s.”.

1248 **Figure 14.** T_{vap}-GC-derived pristane/*n*-C₁₇ *versus* phytane/*n*-C₁₈ diagram showing depositional
1249 environment typing.

1250 **Figure 15.** Conceptual scheme showing relevant Rock-Eval-derived TOC, S₂ and HI parameters, as well
1251 as Py-GC-derived concentration of retained oil. The superscripts ^{ma} and ^{im} denote the present-day
1252 conditions for mature and immature samples, respectively, and superscript ⁱⁿⁱ refers to the initial
1253 conditions of the present-day mature samples. “C” represents the GC-derived component
1254 concentration of specific *n*-alkane. The parameters, which can be directly measured are in black, while
1255 the calculated ones are in red. Modified from Cooles et al. (1986).

1256 **Figure 16.** Compositional mass balance calculation based on specific compounds (*n*-alkanes) showing
1257 the average amount of generated and retained hydrocarbons for each interval and for overall
1258 succession without siltstone samples.

1259 **Figure 17.** Rock-Eval S₁, S₂, HI and T_{max} parameters *versus* depth profile of the Zhang 22 well after
1260 Soxhlet extraction. Note that extremely low T_{max} values of eight unextracted siltstones were excluded
1261 in order to display more clear trends of the distributive pattern.

1262 **Figure 18.** Rock-Eval pyrograms showing programmed temperature curves, and hydrocarbons
1263 generation curves before (green solid lines) and after (red stippled lines) the Soxhlet extraction as a
1264 function of time. In order to make a meaningful comparison, the initial signal intensity was normalized
1265 to the weight of rocks (left *y*-axis). The temperature program curves were shown pertinent to the
1266 right *y*-axis.

1267 **Figure 19. (a)** Rock-Eval pyrolytic S₁ of unextracted rocks *versus* thermal solvent-extraction yields; **(b)**
1268 unextracted S₁ values association with solvent extract yields *versus* calculated total oil content.

1269 **Figure 20.** Expulsion efficiency calculation based on specific compound (*n*-alkane) showing the
1270 average amount of expelled hydrocarbons, and the curves of expulsion efficiency for each interval
1271 and for overall succession without siltstone samples.

1272 **Figure 21.** Compound-specific (*n*-C₁₇) mass balance calculation showing the amount of generated,
1273 retained and expelled hydrocarbons, as well as the expulsion efficiency through the entire succession.

1274 **Figure 22. (a)** TOC content (wt. %) *versus* Rock-Eval S₁ values, and **(b)** quartz content *versus* Rock-Eval
1275 S₁ values, describing controls of organic richness and quartz content on hydrocarbon retention. **(c)**
1276 calculated S₁ using regression formula considering the organic richness and quartz content *versus*
1277 Rock-Eval S₁ values, and **(d)** calculated S₁ using regression formula involving S₂ values and quartz
1278 content *versus* Rock-Eval S₁ values, showing the contribution of live carbon on petroleum retention.

1279 **Table 1.** Brief classification of investigated the Zhang 22 well succession by Industrial Oilfield Company
1280 and by this study.

1281 **Table 2.** Average mineralogical composition for each investigated interval and for the entire
1282 succession. Note: siltstone samples consist of two Chang 6 samples and six siltstones from interval-1,
1283 hence the average values of interval-1 are excluding siltstones.

1284 **Table 3.** The average results of the unextracted and extracted Rock-Eval data, and the solvent
1285 extraction yields for each interval.

1286 **Table 4.** Bulk chemical fraction yields for selected samples. The average values for each group are
1287 shown in bold and italic.

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