Supplementary Material for

Using nanoindentation to quantify the mechanical profile of Wufeng-Longmaxi formation shale in Southwest China: Link to sedimentary conditions

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Table S1. Composition and pore parameters of shale samples (after Zheng et al. (2018)).

Sample	Depth (m)	TOC （wt. %)	Quartz (%)	Clay (%)	Feldspar (%)	Calcite (%)	Dolomite (%)	Pyrite (%)	Porosity (%)	PV_{total} (10^{-3} mL/g)	SA_{total} (10^{2} m^2/g)
SQ-11	11.8	0.53	20.8	54.1	14.5	6.5	2.3	2	/	/	/
SQ-17	17.5	0.91	22.7	49.6	15.9	7.6	2.1	2.1	/	/	/
SQ-20	20.8	1.36	24.4	46.6	16.8	4	1.7	6.4	2.80	24.1	19.9
SQ-27	27.6	1.59	28.3	42.9	19.6	4.4	2.6	2.3	/	/	/
SQ-30	30.6	1.51	26.3	46.2	17	5.7	2.6	2.1	2.10	21.4	19.2
SQ-40	40.8	1.46	27.7	45.6	16.6	5.3	3	1.9	1.30	22.3	18.9
SQ-45b	45.8	1.10	25.1	48.1	16.1	3.1	2.0	2.0	/	/	/
SQ-50	50.5	0.95	25.2	51.1	15.1	3.7	2.8	2.1	1.80	23.5	18.5
SQ-61b	61.7	1.18	27	42.4	20.1	2.9	2.2	5.3	2.17	24.3	18.8
SQ-62	62.3	1.44	27.3	44.2	20.4	3.7	2.7	1.6	/	21.0	19.3
SQ-65	65.2	2.23	24.5	43.6	19.5	3.6	2.3	6.5	3.37	27.8	24.9
SQ-68	68	2.32	29.3	43.5	17.5	4.3	3.6	1.7	/	30.1	27.4
SQ-70a	70.2	2.38	32.8	41.0	17.9	3.3	3	1.9	3.29	25.3	24.1
SQ-75b	75.6	3.14	32.5	38.2	16.2	3.7	3	6.5	2.77	31.0	29.1
SQ-77b	77.7	2.9	29.8	40.7	14.8	6	1.9	6.8	/	/	/
SQ-78	78	2.58	32.4	38.9	16.1	7.9	2.8	1.9	/	/	/
SQ-78b	78.8	2.62	30.4	40.8	18.3	4.4	3.7	2.4	/	27.2	25.2
SQ-80b	80.6	3.07	39.6	33.8	13.8	4.3	2	6.5	3.62	27.5	25.7
SQ-81a	81.1	2.71	34.5	38.5	17.3	3.9	3.7	2	/	/	/
SQ-81	81.4	2.79	37.2	36.7	14.8	4.5	4.6	2.2	/	25.9	23.8
SQ-83	83.4	2.68	43.6	30.3	15.2	3.2	2.4	5.4	1.50	23.0	20.9
SQ-85	85.6	6.53	44.4	31.2	13.3	2.9	2.2	5.9	4.12	40.9	42.0

SQ-86	86.4	4.41	51.5	23.1	12.5	3.2	2.2	1.8	4.66	30.6	35.2
SQ-87	87.4	4.2	53.3	29.1	10.6	3.6	2.1	1.3	6.38	41.4	28.7
SQ-88	88.3	3.45	29.3	48.1	14.5	2.8	2.2	3.1	/	/	/
SQ-89	89.1	3.29	34.4	45.9	13.6	2.7	1.8	1.5	2.94	40.3	27.8
SQ-90	90	1.30	22.7	48.3	19.4	3.1	5	1.5	/	/	/

Note: PV_{total}=the total nanopore volume. SA_{total}=the total nanopore surface areas. The mineral content is the volume percentage.

Table S2. The results of major oxides and related parameters characteristics of shale samples (after Zheng et al. (2018)).

Sample	Depth (m)	Al_2O_3 (%)	CaO (%)	Fe_2O_3 (%)	K_2O (%)	MgO (%)	Na_2O (%)	MnO (%)	TiO2 (%)	SiO_2 (%)	Excess SiO_2 (%)	CIA (%)	PIA (%)
SQ-20	20.8	15.1	3.44	6.37	3.68	2.41	0.94	0.03	0.72	59.15	12.19	68.1	78.2
SQ-30	30.6	14.57	3.73	6.2	3.54	2.57	0.96	0.04	0.69	58.63	13.32	67.5	77.3
SQ-45b	45.8	15.78	2.22	6.26	3.94	2.69	0.83	0.04	0.70	59.94	10.86	69.3	80.8
SQ-50	50.5	15.9	2.03	6.24	4.02	2.78	0.73	0.04	0.68	60.02	10.57	70.2	82.8
SQ-65	65.2	15.36	2.22	6.41	3.84	2.48	1.2	0.03	0.71	59.15	11.38	65.4	73.9
SQ-70a	70.2	12.39	2.62	6.05	3.13	2.04	0.98	0.03	0.58	62.64	24.11	65.2	73.6
SQ-75b	75.6	12.02	3.42	4.87	3.19	2.04	0.76	0.03	0.59	62.12	24.74	66.8	77.4
SQ-80b	80.6	9.95	2.91	4.13	2.62	1.42	0.67	0.02	0.47	68.64	37.70	66.3	76.3
SQ-83	83.4	11.9	2.07	5.26	3.22	1.66	0.89	0.02	0.58	63.55	26.54	64.9	74.2
SQ-85	85.6	7.74	2.01	3.2	2.1	1.2	0.62	0.02	0.39	70.2	46.13	64.2	72.8
SQ-86	86.4	5.55	2.44	3.03	1.49	1.14	0.39	0.03	0.27	76.19	58.93	65.7	75.4
SQ-87	87.4	5.72	3.02	2.34	1.5	0.98	0.41	0.03	0.27	76.32	58.53	65.8	75.2
SQ-88	88.3	8.38	3.73	3.2	2.28	1.68	0.43	0.05	0.40	69.1	43.04	68.3	80.7
SQ-89	89.1	15.65	3.56	4.36	4.21	2.93	0.92	0.05	0.76	56.82	8.15	67.3	78.5

CIA = 100 × Al_2O_3 / (Al_2O_3 + CaO* + Na_2O + K_2O;PIA = 100 × (Al_2O_3 - K_2O) / ((Al_2O_3 - K_2O) + CaO* + Na_2O)). The units of the oxides used in these calculations are molar masses. CaO* refers specifically to the CaO content in silicate minerals. Since the CaO content in silicate minerals is often comparable to that of Na_2O, a correction method is applied: if the molar amount of CaO is greater than that of Na_2O, CaO = Na_2O; conversely, if the molar amount of CaO is less than that of Na_2O, no correction for CaO is required.

Table S3. Micromechanical parameters of shale samples.

Sample	Depth (m)	E (GPa)				H (GPa)				K_c (MPa • m $^{0.5}$)				B (μm^{-1})			
		X1		X3		X1		X3		X1		X3		X1		X3	
		Ave.	Std.	Ave.	Std.	Ave.	Std.	Ave.	Std.	Ave.	Std.	Ave.	Std.	Ave.	Std.	Ave.	Std.
SQ-11	11.8	14.3	1.7	25.2	2.3	0.36	0.09	0.53	0.11	0.51	0.13	0.69	0.14	23.8	12.0	26.2	11.8
SQ-17	17.5	12.8	2.0	18.8	3.3	0.31	0.10	0.41	0.12	0.44	0.13	0.56	0.19	18.2	6.9	25.7	9.0
SQ-20	20.8	22.2	5.1	24.2	3.5	0.64	0.30	0.78	0.23	0.78	0.27	0.87	0.20	24.8	11.5	26.6	11.0
SQ-27	27.6	18.4	4.2	25.7	5.8	0.56	0.18	0.82	0.34	0.69	0.21	0.97	0.22	25.4	10.0	29.0	11.1
SQ-30	30.6	19.8	3.0	25.7	3.2	0.71	0.25	0.82	0.19	0.82	0.17	0.95	0.19	21.3	9.7	24.2	8.8
SQ-40	40.8	20.5	2.3	28.0	4.3	0.73	0.28	0.85	0.29	0.78	0.21	0.88	0.19	26.5	9.2	28.1	8.2
SQ-45b	45.8	23.2	3.7	27.4	2.3	0.72	0.17	0.75	0.11	0.81	0.20	0.91	0.17	24.3	10.1	26.8	9.0
SQ-50	50.5	21.8	2.8	29.1	3.9	0.72	0.16	1.00	0.23	0.83	0.17	1.01	0.26	24.8	8.3	32.2	10.4
SQ-61b	61.7	26.0	3.4	29.0	5.3	1.02	0.21	1.06	0.56	0.96	0.36	1.01	0.37	28.5	9.1	30.3	11.2
SQ-62	62.3	21.3	3.8	30.6	4.3	0.79	0.29	0.98	0.48	0.77	0.25	1.06	0.35	22.7	6.8	28.7	11.0
SQ-65	65.2	24.9	6.0	31.3	4.2	0.92	0.51	0.96	0.34	1.02	0.39	1.08	0.34	27.9	11.7	29.4	10.0
SQ-68	68	19.4	3.3	27.7	4.6	0.73	0.24	0.92	0.48	0.77	0.18	0.92	0.26	26.2	18.9	31.6	10.8
SQ-70a	70.2	21.5	5.2	26.4	5.1	0.88	0.52	0.88	0.44	0.92	0.38	0.94	0.23	24.6	8.7	28.1	9.4
SQ-75b	75.6	24.1	3.8	27.7	4.8	0.94	0.48	0.98	0.29	0.97	0.34	1.00	0.27	25.6	8.6	28.7	6.6
SQ-77b	77.7	21.4	3.5	28.2	3.3	0.80	0.27	0.89	0.12	0.78	0.18	0.92	0.17	30.5	9.6	31.8	13.0
SQ-78	78	24.4	3.2	29.8	2.9	0.97	0.30	1.07	0.33	0.95	0.25	0.95	0.19	29.8	11.3	36.0	9.2
SQ-78b	78.8	23.2	3.0	29.4	3.2	0.84	0.25	0.95	0.41	0.78	0.21	0.90	0.31	33.8	12.8	37.3	10.5
SQ-80b	80.6	26.9	4.6	33.1	4.1	1.20	0.49	1.32	0.48	1.01	0.31	1.06	0.27	37.5	14.5	40.5	11.2
SQ-81a	81.1	24.1	3.1	33.0	4.0	1.10	0.28	1.34	0.54	0.85	0.23	1.07	0.33	37.1	12.8	39.6	13.5
SQ-81	81.4	23.3	3.1	30.6	3.7	1.00	0.30	1.41	0.45	0.84	0.23	1.03	0.33	38.2	14.5	42.6	14.3
SQ-83	83.4	27.1	4.2	30.4	3.7	1.41	0.49	1.70	0.73	1.03	0.28	1.04	0.28	44.7	13.3	47.9	11.8

SQ-85	85.6	29.0	8.3	39.2	9.8	0.91	0.47	1.61	0.68	0.80	0.30	1.17	0.40	43.9	12.5	48.2	12.6
SQ-86	86.4	30.5	2.9	32.0	3.8	1.53	0.38	1.72	0.45	1.06	0.20	1.09	0.21	45.1	15.1	47.5	9.9
SQ-87	87.4	31.6	3.8	35.9	3.7	2.43	0.68	2.93	0.84	1.25	0.23	1.43	0.26	49.3	10.2	52.4	9.6
SQ-88	88.3	23.0	5.0	28.4	5.1	0.94	0.49	1.06	0.42	0.97	0.29	1.06	0.22	24.4	8.4	29.3	10.2
SQ-89	89.1	20.2	2.0	26.2	3.2	0.78	0.13	0.81	0.26	0.81	0.12	0.91	0.22	25.0	4.8	28.3	8.8
SQ-90	90	17.1	2.1	25.3	3.3	0.44	0.11	0.64	0.16	0.66	0.16	0.86	0.17	20.1	7.4	23.5	6.7

Text S1: Calculation of fracture toughness and brittleness index

In this study, we used the energy-based method to calculate the fracture toughness of coal and its macerals (Liu et al. 2016, Liu 2015, Manjunath and Jha 2019a, b). In this method, the total energy (U_t) is a sum of the elastic energy (U_e), fracture energy (U_{frac}), and pure plastic energy (U_{pp}).

$$U_t = U_e + U_{pp} + U_{frac} \tag{S1}$$

The elastic energy (U_e) and total energy (U_t) are derived from the *P*-*t* curve using the following equations:

$$U_e = \int_{h_f}^{h_{max}} \alpha \left(h - h_f\right)^m dh \tag{S2}$$

$$U_t = \int_{h_f}^{h_{max}} Kh^n dh + P_{max}\left(h_{max} - h_0\right) \tag{S3}$$

where h_f represents the residual displacement, h_0 is the displacement value at the beginning of the holding stage, and K, α, *n*, and *m* are the fitting values that are determined based on fitting the loading and unloading curves using the following equations.

$$P = \mathrm{K}\ h^n \text{ (loading stage)} \tag{S4}$$

$$P = \alpha\ (h - h_f)^m \text{ (unloading stage)} \tag{S5}$$

Then, the pure plastic energy U_{pp} can be obtained (Liu et al. 2016):

$$\frac{U_{pp}}{U_t} = 1 - \frac{(1+n)(1-\frac{h_f}{h_{max}})}{1+m} \tag{S6}$$

However, Equation (S6) does not take into account the displacement that occurs during the holding stage, which can lead to an overestimation of the fracture toughness value (Zeng et al. 2017). Therefore, a revised equation is introduced that incorporates the influence of the holding stage (Zeng et al. 2017):

$$\frac{U_{\mathrm{pp}}}{U_{\mathrm{t}}}=1-\frac{(1+n)(1-\frac{h_{\mathrm{f}}}{h_{\max}})}{(1+m)(1+n-n\frac{h_0}{h_{\max}})} \tag{S7}$$

Hence, we used Eq. (S7) to obtain fracture toughness in this work. Then, the fracture energy (U_{frac}) can be calculated as follows:

$$U_{\mathrm{frac}}=U_{\mathrm{t}}-U_{\mathrm{e}}-U_{\mathrm{pp}} \tag{S8}$$

Then, G_c, the critical energy release rate, is determined as:

$$G_c=\frac{U_{\mathrm{frac}}}{A_{\max}} \tag{S9}$$

where $A_{\max}$ is the maximum crack area and can be calculated as:

$$A_{\max}=24.5h_{\max}^2 \tag{S10}$$

Finally, the fracture toughness, K_c, can be determined as:

$$K_{\mathrm{c}}=\sqrt{G_{\mathrm{c}}E_{\mathrm{r}}} \tag{S11}$$

After we obtained K_c, the brittleness index (B) based on the mechanical properties can be calculated as (Lawn and Marshall 1979):

$$B=\frac{HE}{K_{\mathrm{c}}} \tag{S12}$$

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