

Supplementary file

The effect of kerogen content and maturation on physical properties of oil and gas shales

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Appendix A: Kerogen properties and its multi-scale distribution in shales

Table S1 summarizes results of various experimental studies of different kerogen properties, which are helpful for (1) interpreting variations in the properties of oil and gas shales with logging or laboratory data via well-known approaches, including the theoretical modeling (Mavko et al., 2020), (2) conducting parametric studies during numerical modeling the process of conversion and extraction of hydrocarbons from kerogen-bearing rocks. Natural causes (the heterogeneity of the petrographic composition and changes in degree of OM catagenesis related to geological conditions) and technogenic causes (uncertainty of measurements, the variety of techniques to isolate kerogen and/or to study its property) lead to a wide range of kerogen physical properties. With increasing maturity, the kerogen pore volume and the specific surface area increase (Craddock et al., 2018; Valenza et al., 2013), while the chemical composition changes (hydrogen-rich functional groups are separated from the initial kerogen and enriched with aromatic carbon structures, see Tissot and Welte, 1984), which affects the density and other physical properties of kerogen.

Table S1. Ranges of changes in kerogen properties based on the results of generalization of published data.

Kerogen properties	Range	References
Mechanical and elastic		
Young's modulus (E)	0.1-16 ^A GPa	(Zeszotarski et al., 2004; Ahmadov, 2011; Kumar et al., 2012; Shukla et al., 2013; Alstadt et al., 2015; Emmanuel et al., 2016; Li et al., 2018; Khatibi et al., 2018; Charlton et al., 2021)
Poisson's ratio (ν)	0.14-0.42	(Mavko et al., 2020)
Bulk modulus (K)	3-11 GPa	(Ahmadov, 2011; Yan and Han, 2013; Yenugu, 2014; Schoen, 2015; Mavko et al., 2020)
Shear modulus (μ)	1.8-5 GPa	(Wu and Firoozabadi, 2020)
Compressive strength (σ_c)	100.1-186.1 MPa*	
Tensile strength (σ_t)	72.9-133.3 MPa*	
Cohesion	42.8-79.2 MPa*	
Friction coefficient	0.153-0.191*	
Hardness	0.2-1.3 GPa	(Zeszotarski et al., 2004; Alstadt et al., 2015; Wang et al., 2024)

Thermal

Thermal conductivity (λ)	0.08-0.64 W/(m·K)	(Barshchevsky et al., 1963; Popov, 2019; Gabova, 2022)
Volumetric heat capacity (C)	1.45-1.65 ^D MJ/(m ³ ·K)	(Popov, 2019)
Specific heat capacity (c)	1.465-1.5 ^E J/(g·K)	(Zelenin and Ozerov, 1983; Berkovich et al., 2000; Waples and Waples, 2004)
Coefficient of linear thermal expansion (α)	104-598 $\times 10^{-6}$ K ⁻¹	(Smith and Johnson, 1976; Kaevand and Lille, 2005; Zhang et al., 2007)

Electric

Dielectric permittivity (ϵ)	1.85-3.2	(Jagadisan and Heidari, 2020)
Electrical resistivity (Rt)	10^3 - 10^{11} Ohm·m	(Yang et al., 2016)

Density, porosity, SSA

Density (ρ)	1.04-1.79 ^B g/cm ³	(Zelenin and Ozerov, 1983; Guidry et al., 1995; Ward, 2010; Alfred and Vernik, 2013; Schoen, 2015; Dang et al., 2016; Cheshire et al., 2017; Craddock et al., 2018)
Porosity (ϕ)	up to 0.57 ^C	(Vasiliev et al., 2015; Mavko et al., 2020)
Specific surface area (SSA)	26-403 ^F m ² /g	(Suleimenova et al., 2014; Cheshire et al., 2017)

^A The data by Eliyahu et al. (2015) are not taken into account, because the estimate of the upper bound of the Young's modulus (25 GPa) is very different from the estimates of other researchers.

^B The data by Kinghorn and Rahman (1983) are not taken into account, see Fig. 1(a).

^C The porosity of kerogen increases with increasing degree of its thermal transformation (maturity); $\phi = \phi_{\max} TR$, where TR is the transformation ratio of OM, while the maximal porosity $\phi_{\max}$ can exceed 57% for Type-I kerogen, see examples in (Mavko et al., 2020).

^D Without accounting for the value of 1.8 MJ/(m³·K) from (Waples and Waples, 2004).

^E Without accounting for the range 1.82-2.86 J/(g·K) if temperature changes from 25 to 350 °C (Berkovich et al., 2000).

^F The range 709–921 m²/g (Derkowski and Bristow, 2012) is not taken into account, because it significantly exceeds the estimates of other researchers.

* Due to the lack of experimental data, results of molecular dynamics simulation are shown.

The physical properties of kerogen differ significantly from those of most minerals of kerogen-bearing rocks (with some exceptions, e.g., for kaolinite): kerogen is significantly less dense and thermally conductive, characterized by lower values of volumetric heat capacity,

dielectric constant, shear modulus, bulk modulus, compressive strength and hardness, high values of thermal coefficient of linear expansion and electrical resistivity (Table S1). Errors in assumed kerogen properties in common wellbore logging interpretations can result in gross errors (e.g., 25%-40 %) in the resulting resource estimates (Craddock and Sauerer, 2022).

The physical properties of oil and gas shales depend not only on the properties and content of kerogen (and generated products), but also on the distribution of organic matter in the mineral matrix (Figs. S1(a) and S1(b)). There are distributions nonuniformly and chaotically (dotted, in the form of clusters, spots) or laminate, with layers and elongated lenses of different thicknesses (Vandenbroucke and Largeau, 2007). For the example in Fig. S1, the thermal anisotropy for a sample with a layered kerogen distribution is approximately two times higher than for a sample with a dotted distribution.

It is important that the textural features can vary significantly even within a small depth range of the same well, which is further complicated by a significant multi-scale variation in the content of organic matter (Fig. S1(c), where the registration of multiscale variations in the thermal conductivity component parallel to bedding along wells with a spatial resolution of 1 mm was carried out using the method of continuous thermophysical profiling (Popov, 2019)). Kerogen-enriched rocks are usually represented as a transversely isotropic medium with a vertical axis of symmetry perpendicular to the stratification and preferred orientation of kerogen layers/lenses and clay particles (the so-called VTI or “vertical transversely isotropic” medium) (Vernik and Milovac, 2011).

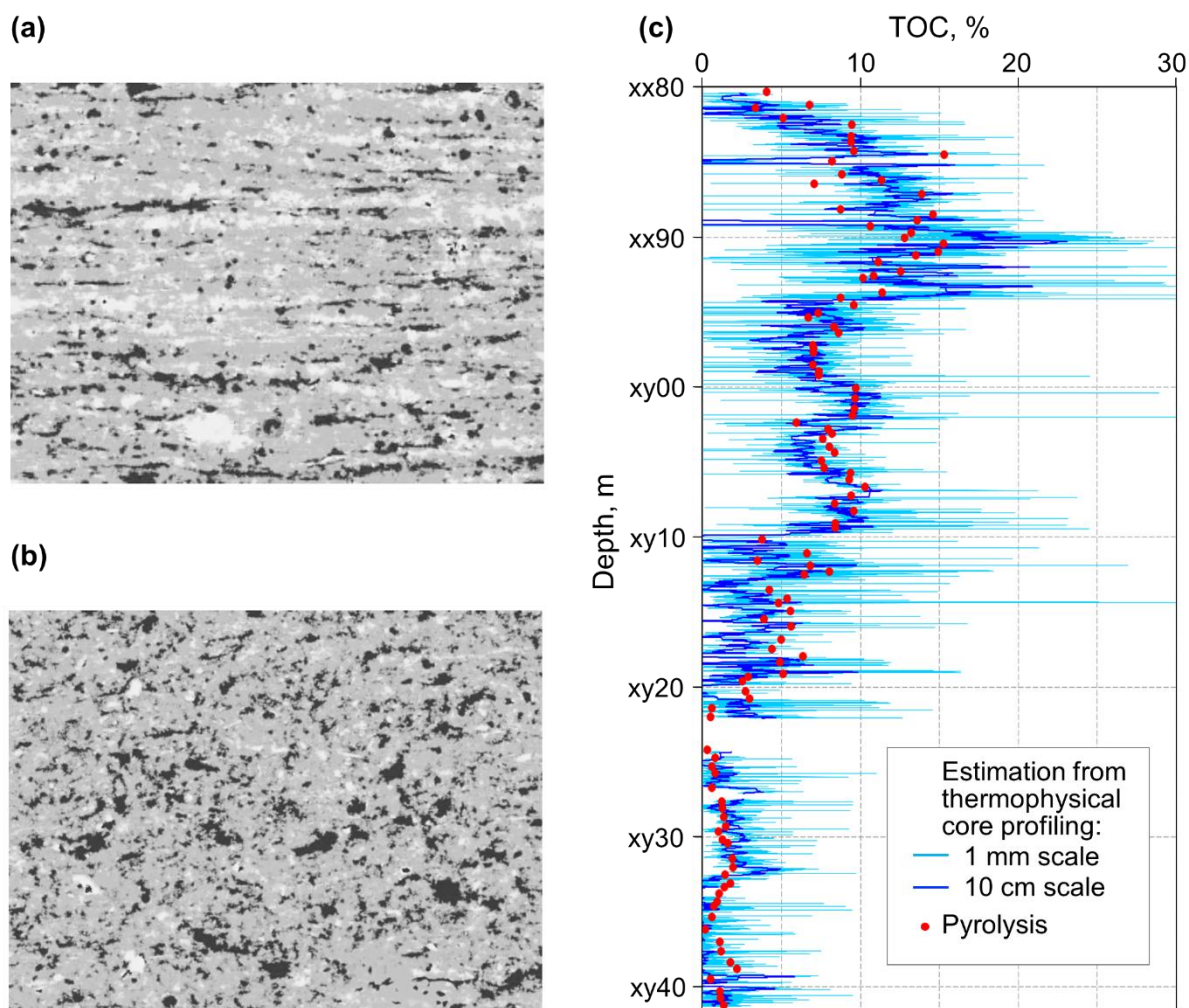


Fig. S1. Images of two microtextural types of kerogen distribution (shown in black) in Bazhenov Fm. rocks based on the thin section analysis of two samples from one well: (a) in the form of layers and elongated lenses along bedding, and (b) dotted, in the form of spots and clusters; a modification of images from (Gutman et al., 2017). (c) Example of a significant multi-scale variation of the total organic carbon content within the Bazhenov Fm., determined by the results of continuous thermophysical core profiling with a spatial resolution of 1 mm (cyan curve), after averaging the results in a sliding 10 cm window (blue curve), and according to pyrolytic studies (red markers) (Popov, 2019).

Appendix B: Regression equations for different formations

The Appendix B contains tables describing the properties of the physical properties of kerogen and organic-rich shales, depending on the degree of thermal maturity (the vitrinite reflectance R_o , %), the total content of organic carbon (TOC, mass %), the volume fraction of

the organic presence in the rock, etc. in Figs. 1, 4, 5, 8(b), 10-13.

Table S2. Dependences of kerogen density (ρ_k , g/cm³) on the level of thermal maturity (R_o , %) for organic-rich shales.

Formation	OM type	Regression equation*	References
Woodford, USA	II+III, III	$\rho_k = 0.987 + 0.313R_o$ ($r=0.93$)	(Dang et al., 2016)
	II	$\rho_k = 1.303 + 0.264\ln(R_o)$ ^a	(Craddock et al., 2018)
Not disclosed	n/a	$\rho_k = 1.293R_o^{0.2}$	(Alfred and Vernik, 2013)
Marcellus, USA	n/a	$\rho_k = 0.972 + 0.342R_o$	(Ward, 2010)
Mix-1 ^b , USA	n/a	$\rho_k = 0.963 + 0.349R_o$ ($r=0.96$)	(Guidry et al., 1995)
Mix-2 ^c , USA	II	$\rho_k = 1.311 + 0.247\ln(R_o)$ ($R^2=0.94$)	(Cheshire et al., 2017)

* The correlation coefficient r for a linear equation or the coefficient of determination R^2 for a nonlinear equation are shown in parentheses (where possible).

^a The equation is a digitized curve from the work (Craddock et al., 2018).

^b Ohio (L.Huron and Cleveland), Norwood/Antrim, and Barnett shales according to Guidry et al. (1995).

^c The regression equation is obtained based on published tabular data (Cheshire et al., 2017) for samples of Woodford, Eagle Ford, New Albany, Bakken, and Marcellus shales (including some not disclosed data).

Table S3. Dependences of bulk density (ρ , g/cm³) on the total organic carbon (TOC, mass %) for organic-rich shales.

Formation	OM type	Regression equation (correlation coefficient)	References
Antrim, USA	n/a	$\rho = 2.60 - 0.03\text{TOC}$ ($r=-0.91$)	(Decker et al., 1993)
Bazhenov, Russia	II	$\rho = 2.545 - 0.0270\text{TOC}$ ($r=-0.85$) ^a	(Gabova, 2022)
Bakken, USA	n/a	$\rho = 2.648 - 0.0275\text{TOC}$ ($r=-0.95$) ^b	(Vernik and Liu, 1997)
	n/a	$\rho = 2.701 - 0.0358\text{TOC}$ ($r=-0.94$) ^a	(Yenugu and Han, 2013)
Vaca Muerta, Argentina	II	$\rho = 2.659 - 0.0351\text{TOC}$ ($r=-0.89$) ^c	(Deitrich, 2015)
Domanik, Russia	n/a	$\rho = 2.57 - 0.029\text{TOC}$ ($r=-0.95$) ^a	(Yusupova et al., 2019)

Kimmeridge, UK	<i>n/a</i>	$\rho = 2.74-0.061\text{TOC}^a$	(Sondergeld et al., 1999)
Longmaxi-Wufeng, China	<i>n/a</i>	$\rho = 2.737-0.0620\text{TOC}$ ($r=-0.90$) ^c	(Huang et al., 2015)
Qingshankou, China	I,II	$\rho = 2.78-0.05\text{TOC}$ ($r=-0.90$)	(Tan, 2020)
Not disclosed, LOM 6-7 ($R_o \approx 0.42\%$ - 0.48 %)	<i>n/a</i>	$\rho = 2.386-0.0250\text{TOC}$ ($r=-0.80$) ^a	(Passey et al., 1990)
Not disclosed, LOM 7 ($R_o \approx 0.48\%$)	<i>n/a</i>	$\rho = 2.568-0.0345\text{TOC}$ ($r=-0.92$) ^a	(Passey et al., 1990)

^a The regression equation is obtained based on published tabular data or curves (after its digitizing).

^b The regression equation is obtained based on published tabular data after the volume fraction of kerogen is converted to the mass fraction using formula (1) with $\rho_k=1.25 \text{ g/cm}^3$ and $w=0.8$.

^c The coefficients of the equation are recalculated from the published dependence $\text{TOC}(\rho)$.

Table S4. Dependences of the porosity ϕ (%) on TOC (mass %) for rocks of organic-rich shales with indication of the thermal maturity level.

<i>Formation, regression equation (correlation coefficient)</i>	<i>R_o, %</i>	<i>References</i>
<i>Bazhenov, Russia</i>		
$\phi = 0.54 + 0.62\text{TOC}$ ($r=0.81$)	0.85-1.55	(Kalmykov and Balushkina, 2017)
<i>Marcellus, USA</i>		
$\phi = 2.75 + 1.24\text{TOC}$ ($r=0.94$) ^a	1.0	(Milliken et al., 2013)
$\phi = 0.95 + 1.45\text{TOC}$ ($r=0.91$) ^a	2.1	
<i>Eagle Ford, USA</i>		
$\phi = 3.95 + 0.66\text{TOC}$ ($r=0.44$) ^a	0.68-1.5	(Quirein et al., 2013)
<i>Doig Phosphate, Canada</i>		
$\phi = 1.85 + 0.36\text{TOC}$ ($r=0.83$)	<i>n/a</i>	(Jarvie, 2012)
<i>Longmaxi, China</i>		
$\phi = 4.57 + 2.04\ln(\text{TOC})$ ($r=0.93$)	2.0-2.3	(Zhao et al., 2024)
$\phi = 1.96 + 0.36\text{TOC}$ ($r=0.92$)	2.32-2.42	(Tang et al., 2016)
<i>Niutitang, China</i>		
$\phi = 1.68 + 0.33\text{TOC}$ ($r=0.97$)	3.49-3.66	(Tang et al., 2016)
<i>Qijia Gulong, China</i>		
$\phi = -0.53 + 3.75\text{TOC}$ ($r=0.93$)	1.2-1.6	(Zhao et al., 2024)
<i>Qiongzhusi, China</i>		
$\phi = 1.53 + 0.66\text{TOC}$ ($r=0.97$)	2.5-2.8	(Zhao et al., 2024)
$\phi = 1.65 + 0.94\ln(\text{TOC})$ ($r=0.87$)	2.8-3.1	

^a The equation is obtained based on digitized data.

Table S5. Dependences of the methane adsorption capacity (AC, cm³/g) on TOC (mass %) of dry and moisture equilibrated organic-rich shales with indication, if available, the OM type and the thermal maturity level.

Formation, regression equation (correlation coefficient, if available)	OM type	R_o range, %	References
<i>Buckinghorse, Canada</i> AC = 0.128TOC + 0.159 ($r=0.82$)*	<i>n/a</i>	<i>n/a</i>	(Chalmers and Bustin, 2008)
<i>Longmaxi, China</i> AC = 0.568TOC + 0.035 ($r=0.97$)	I	2.32-2.42	(Tang et al., 2016)
<i>Longmaxi and Niutitang, China</i> Moist: AC = 0.484TOC + 0.291 ($r=0.99$)*	<i>n/a</i>	2.5-3.5	(Tan et al., 2014)
<i>Niutitang, China</i> AC = 0.654TOC + 0.415 ($r=0.99$)	I	3.49-3.66	(Tang et al., 2016)
<i>Mix-1</i> Dry: AC = 0.441TOC + 1.187* Moist: AC = 0.264TOC + 0.224*	<i>n/a</i>	<i>n/a</i>	(Yang et al., 2017)
<i>Mix-2</i> Dry: AC = 0.25TOC + 1.36 ($r=0.75$) Moist: AC = 0.15TOC + 0.21 ($r=0.79$)	<i>n/a</i>	<i>n/a</i>	(Klewiah et al., 2020)
<i>Qinshui Basin shales, China</i> Dry: AC = 0.387TOC + 1.166 ($r=0.96$) Moist: AC = 0.379TOC + 0.375 ($r=0.94$)	III	2.5-3.0	(Sun et al., 2022)

* The equation is obtained based on published tabular or digitized data.

Table S6. Dependences of the coefficient of linear thermal expansion α (10⁻⁶ K⁻¹) on TOC (mass %) of organic-rich shales.

Formation	OM type	Regression equation (determination coefficient)	References
Bazhenov, Russia	II	$\alpha = 0.09\text{TOC}^2 + 0.34\text{TOC} + 7.88$ ($R^2=0.79$)	(Gabova et al., 2020a)
Yanchang, China	I, II	$\alpha_{\perp} = 7.94\exp(0.053\text{TOC})$ ($R^2=0.85$)* $\alpha_{\parallel} = 7.94\exp(0.034\text{TOC})$ ($R^2=0.90$)*	(Li et al., 2023)

* The equation is obtained based on digitized data (Li et al., 2023).

Table S7. Dependences of elastic moduli, namely Young's modulus (E) and Poisson's ratio (ν), on TOC (mass %) of organic-rich shales.

Formation	OM type	R _o , %	Regression equation (correlation or determination coefficient)	References
Bazhenov, Russia	n/a	n/a	E = 63.81–2.568TOC (r=–0.95) ^{a,b} E _⊥ = 38.06–1.782TOC (r=–0.78) ^{a,b} v = 0.147+0.0045TOC (r=0.70) ^{a,b} v _⊥ = –0.013+0.0203TOC (r=0.93) ^{a,b}	(Vernik and Liu, 1997)
	II	0.65-0.85	E = 33.59exp(–0.074TOC)	(This study)
	n/a	n/a	E = 76.18–15.46ln(TOC) (R ² =0.91) ^{a,b} E _⊥ = 56.47–13.14ln(TOC) (R ² =0.77) ^{a,b}	(Vernik and Liu, 1997)
	Bakken, USA	n/a	n/a	E = 67.23–13.19ln(TOC) (R ² =0.84) ^a E _⊥ = 79.77–20.01ln(TOC) (R ² =0.88) ^a
Vaca Muerta, Argentina		II	Oil window	E = 57.14exp(–0.091TOC) (R ² =0.79)
	E _⊥ = 36.92exp(–0.085TOC) (R ² =0.61)			
Woodford, USA	I, II	~1.48	E = 147.96–31.57ln(TOC) (R ² =0.76) v = 0.202–0.0103TOC (r=–0.52)	(Harris et al., 2019)
		~0.71	E = 47.56–13.02ln(TOC) (R ² =0.27) v = 0.286–0.028ln(TOC) (R ² =0.14)	
			n/a	n/a
	Lucaogou, China	I	0.72-0.96	v = 0.268–0.0045TOC (r=–0.72)
Niutitang, China	I	2.27-4.42	v = 0.27–0.01TOC (r=–0.56)	(Wang et al., 2016)
Nanoindentation tests:				
Mix ^c , USA	n/a	n/a	E = 58.5–3.3TOC (r=–0.69)	(Kumar et al., 2012)
Longmaxi, China	n/a	n/a	E = 64.53–8.718TOC (r=–0.93)	(Long et al., 2021)

^a The equation is obtained based on published tabular data.

^b The TOC values were recalculated from the volume fraction according to Eq. (1) with a kerogen density of 1.25 g/cm³ and a carbon fraction of 0.8. Elastic moduli were calculated according to Eq. (2).

^c Mix of Barnett, Woodford, Eagle Ford, Ordovician, Haynesville shales; estimates of the Young's modulus are obtained under the assumption that the Poisson's ratio is 0.3.

Table S8. Dependences of the uniaxial compressive strength (σ_c) and the tensile strength (σ_t) on the volume content of organic matter (V_k) for organic-rich shales.

Formation	Regression equation (correlation or determination coefficients)	References
Bazhenov, Russia	$\sigma_c = 99.12 - 1.00V_k$ ($r=-0.87$) ^a	(Kalmykov and Balushkina, 2017)
Bowland, UK and Posidonia, Germany	$\sigma_c = 382.3\exp(-0.147V_k)$ ($R^2=0.92$) ^b	(Herrmann et al., 2018)
Green River, Colorado	$\sigma_{c\parallel} = 127.73 - 1.1215V_k$ ($r=-0.81$)	(Dusseault et al., 1983) ^c
Mahogany zone, USA	$\sigma_{c\perp} = 161.60 - 1.5415V_k$ ($r=-0.86$)	(Dusseault et al., 1983) ^d
Utah	$\sigma_t = 14.78 - 0.0928V_k$ ($r=-0.75$)	(Dusseault et al., 1983) ^d
Green River, Tipton member, USA	$\sigma_t = 13.64 - 0.1211V_k$ ($r=-0.75$)	(Dusseault et al., 1983) ^e
Devonian oil shales, USA	$\sigma_c = 91.27 - 0.709V_k$ ($r=-0.86$)	(Dusseault et al., 1983) ^e
Tennessee	$\sigma_t = 23.16 - 0.3516V_k$	(Dusseault et al., 1983) ^f
Ohio	$\sigma_t = 15.279 - 0.07836V_k$ ($r=-0.78$)	(Chong et al., 1984)
	$\sigma_t = 10.996 - 0.1818V_k$ ($r=-0.80$)	

^a To compare with other data, the original equation $\sigma_c = 99.117 - 2.2167M_k$ ($r=0.87$) was transformed: the volume content V_k of OM was calculated from its mass content M_k , assuming that the ratio of rock density to kerogen density is ~ 2.22 .

^b The equation is obtained based on published tabular data.

^c With reference to (Chong et al., 1980).

^d With reference to (Chong et al., 1982).

^e With reference to (Chong et al., 1976).

^f With reference to (Chong et al., 1979).

Table S9. Dependences of the electrical resistivity R_t (Om·m) of organic-rich shales on TOC (mass %).

Formation	OM type	Regression equation (correlation coefficient)	References
Bazhenov, Russia	II	$R_t = 47.62\text{TOC} - 208.6$ ($r=0.83$) ^a	(Kontorovich, 2002)
Transition zone			
‘Maryanov-Bazhenov Fms.’, Russia		$R_t = 12.99\text{TOC} - 28.4$ ($r=0.88$) ^a	
Qingshankou, China	I, II	$R_t = 0.915\text{TOC} + 5.24$ ($r=0.91$)	(Tan, 2020)
Not disclosed, LOM 7-8 ($R_o \approx 0.48\%-0.56\%$)	n/a	$R_t = 0.248\text{TOC} + 1.82$ ($r=0.74$) ^b	(Passey et al., 1990)
Not disclosed, LOM 9	n/a	$R_t = 6.85\text{TOC} - 6.90$ ($r=0.74$) ^b	

($R_o \approx 0.67\%$) Qiongzhusi Fm. ($R_o \approx 3.3\%-3.7\%$)	n/a	$R_t = 158\exp(-0.38\text{TOC})$ ($R^2=0.76$) ^c	(Liang et al., 2025)
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^a Inverse dependencies to those published in the work (Kontorovich, 2002).

^b The equation is obtained based on published tabular data (Passey et al., 1990).

^c The relationship is converted from the original expression $y = -0.16x + 2.2$ in log scale (Liang et al., 2025).

Table S10. Dependences of the coefficients of thermal anisotropy ($\lambda_{||}/\lambda_{\perp}$) and elastic anisotropy (Thomsen's ε and γ parameters, Young's modulus anisotropy $E_{||}/E_{\perp}$) on TOC and among themselves.

Formation	OM type	Thermal maturity, R_o	Regression equation ^a	References
<i>Dependencies of $\lambda_{ }/\lambda_{\perp}$, ε, γ, and $E_{ }/E_{\perp}$ on TOC (mass %)</i>				
Bazhenov, Russia			$\lambda_{ }/\lambda_{\perp} = 1.067\exp(0.0233\text{TOC})$ ($R^2=0.41$)	
Oilfield 1	II	0.65%-0.85%	$\varepsilon = 0.014\text{TOC} - 0.024$ ($r=0.65$) $\gamma = 0.022\text{TOC} - 0.089$ ($r=0.76$) $E_{ }/E_{\perp} = 0.035\text{TOC} + 0.88$	(This study)
Oilfield 2	II	0.55%-0.65%	$\lambda_{ }/\lambda_{\perp} = 0.950\exp(0.0323\text{TOC})$ ($R^2=0.77$)	
Bakken, USA	n/a	n/a	$\varepsilon = 0.020\text{TOC} + 0.097$ ($r=0.65$) $\gamma = 0.032\text{TOC} - 0.014$ ($r=0.72$)	(Vernik and Nur, 1992)
	n/a	0.35%-1.04%	$E_{ }/E_{\perp} = 0.031\text{TOC} + 0.79$ ($r=0.83$) ^b	(Li et al., 2019)
Kimmeridge, UK	n/a	n/a	$\varepsilon = 0.024\text{TOC} + 0.145$ ($r=0.55$) ^c	(Sondergeld et al., 2000)
<i>Dependencies of ε, γ, and $E_{ }/E_{\perp}$ on $\lambda_{ }/\lambda_{\perp}$</i>				
Bazhenov, Russia	II	0.65%-0.85%	$\varepsilon = 0.269\lambda_{ }/\lambda_{\perp} - 0.290$ $\gamma = 0.384\lambda_{ }/\lambda_{\perp} - 0.445$ $E_{ }/E_{\perp} = 0.625\lambda_{ }/\lambda_{\perp} + 0.310$	(This study)

^a The correlation (r) and determination (R^2) coefficients are shown in parentheses for linear and nonlinear dependencies, respectively.

^b The regression equation is obtained based on tabular data for 6 samples with different levels of thermal maturity (Li et al., 2019); the data were obtained by the nanoindentation method.

^c The equation is obtained based on digitized data.

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