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Research paper

Comprehensive polynomial simulation and prediction for Langmuir volume and Langmuir pressure of shale gas adsorption using multiple factors

Jijun Li, Yan Ma, Kaizhan Huang, Shuangfang Lu*, Jianxin Yin, Yanian Zhang

Research Institute of Unconventional Oil & Gas and Renewable Energy, China University of Petroleum (East China), Qingdao 266580, China

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A B S T R A C T

In this study, 32 experimental measurements on the isothermal adsorption of methane for 18 shale samples from China's three largest continental oil basins—Songliao, Bohai Bay, and Ordos basins—were used to construct comprehensive polynomial simulation and prediction models for Langmuir volume and Langmuir pressure. The models were based on shale properties (total organic carbon (TOC) content, amount of residual hydrocarbon S_1, and mineral composition of rocks) and adsorption condition (temperature) using a weighted sum of multiple variables. The influences of various factors were quantitatively characterized, and the prediction accuracy was verified. Langmuir volume is mainly affected by temperature, shale TOC content, amount of residual hydrocarbon, and clay mineral content; Langmuir pressure is mainly affected by clay, carbonate, feldspar and illite content (because shale pore size can be affected by shale mineral composition). Based on the resource potential and the producibility of shale gas, the area suitable for shale gas exploration and development should have high abundance of organic matter (TOC and residual hydrocarbon S_1), low clay mineral content and feldspar content, high conversion rate of montmorillonite to illite (strong diagenesis), and high carbonate content. The comprehensive polynomial prediction model can effectively simulate and predict Langmuir volume and Langmuir pressure, thereby reducing the amount of work necessary for evaluation of shale gas resource potential and economic feasibility.

1. Introduction

The adsorbed phase is one of the main phases of shale gas, and the Langmuir model is a classic model describing the characteristics of shale gas adsorption (Ji et al., 2014, 2015; Chen et al., 2015; Tian et al., 2016; Langmuir, 1918). The Langmuir adsorption isotherm model is a monolayer and equilibrium adsorption model, and the model can be expressed as Equation (1).

$$V = \frac{V_L p}{p_L + p} \tag{1}$$

where V_L (cm^3/g) is Langmuir volume, representing the maximum adsorption of the sample; p_L (MPa) is Langmuir pressure, equal to the pressure at which half of the Langmuir volume is adsorbed; V (cm^3/g) is the adsorption at pressure p. The production curve and recovery factor of shale gas are largely determined by Langmuir volume and Langmuir pressure (Zhang et al., 2015a,b; Zhu et al., 2016; Zhao et al., 2016); a large Langmuir volume represents a strong adsorption capacity of the shale reservoir and a high Langmuir pressure indicates an easy desorption and extraction of shale gas. Currently, Langmuir volume and Langmuir pressure are mainly obtained through data from isothermal adsorption experiments. Since Langmuir volume and Langmuir pressure are affected by many factors, numerous isothermal adsorption experiments are required to reveal the adsorption characteristics of shale in different regions for the evaluation of resource potential and economic feasibility of a large-area shale gas reservoir. However, if a quantitative relationship for Langmuir volume and Langmuir pressure with each factor can be established, Langmuir volume and Langmuir pressure can be predicted, and the shale gas resource potential and economic feasibility can be easily evaluated. There have been useful studies in this area (Ji et al., 2014, 2015; Yang et al., 2015). However, a relatively small number of factors have been

* Corresponding author.
E-mail address: lushuangfang@upc.edu.cn (S. Lu).

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considered in previous studies; only the effect of temperature was considered in the simulation of Langmuir pressure, and only the effect of total organic carbon (TOC) content was considered in the simulation of Langmuir volume (Zhang et al., 2012). Ji et al. (2014, 2015) only explored the effects of TOC content and temperature; Yang et al. (2015) discussed the impact of TOC content and the influence of mineral composition of rocks, but did not consider the impacts of temperature and bitumen. The reasonableness and fitting accuracy of models can be compromised if not all factors are considered. Additionally, previous studies did not validate the accuracy of extrapolated predictions. In this study, a multivariate prediction model was established from a comprehensive study of experimental methane adsorption data of multiple continental shale samples from China in order to achieve better fit and prediction accuracies as well as broader applicability.

2. Experiment

2.1. Sample

In this study, nine continental shale samples from Bohai Bay and Songliao basins were selected, and 15 isothermal adsorption experiments were carried out under different temperatures. At the same time, 17 isothermal adsorption experimental data for 9 samples from nine continental shales in the southeastern Ordos Basin were collected (Table 1). In Bohai Bay Basin, the samples from Well L69 and Well S352 were selected from Palaeogene Shahejie Formation (E_2S) in Jiyang Depression and Liaohe Depression, respectively. Shahejie Formation shale is deep water turbiditic deposit in warm and humid climate with high subsidence rate (Rotimi et al., 2014; Zhang et al., 2016). The Paleozoic carbonate of the North China Craton is one of main provenance rocks for Shahejie Formation in the Jiyang Depression (Wang, 2013), making the shale rich in carbonate minerals and poor in clay minerals (Zhang et al., 2016, Table 1). In Songliao Basin, the samples from Well G271 and Well Y15 were taken from the Cretaceous Nenjiang Formation (K_2n) and Qingshankou Formation (K_2qn), respectively. Deposition of the Qingshankou Formation and Nenjiang Formation took place within a saline-brackish lake under anoxic conditions in the bottom water (Xu et al., 2015). The samples in Ordos Basin were Triassic Yanchang Formation (T_3y) black shales which were formed in the deep or semi-deep freshwater lacustrine environments (Ji et al., 2014; Liu et al., 2016). Yanchang Formation shale has wide range of organic-matter abundance and high clay minerals content (Tang et al., 2014; Liu et al., 2016). The variations of provenance and sedimentary environment induce the difference in properties of samples from different basins/depressions/strata. The properties difference of samples is the condition of establishing comprehensive simulation and prediction model.

3. Methods

All methane adsorption experiments were completed by Banda Petroleum Technology Co., Ltd., and the experimental methods were consistent with those of Ji et al. (2015). Isothermal adsorption experiments were performed using a self-developed high-pressure gas isothermal adsorption-desorption analyzer, which was installed in an oil bath at a constant temperature. The temperature error is controlled within ±0.2 °C, and the accuracy of pressure is 3.51 kPa. In order to reproduce reservoir conditions, the experiments were conducted at reservoir temperature and equilibrium moisture content. The ASTM standard, D1412-07 (ASTM, 2007),

Table 1
Geochemical properties, Langmuir volume and Langmuir pressure of samples.

Basin	No.	Well	Depth (m)	Temperature (°C)	TOC (%)	Tmax (°C)	S_1 (mg/g)	S_2 (mg/g)	Mineral contents (%)				Illite content in clay mineral (%)	V_L (cm^3/g rock)	P_L (MPa)
									Clay mineral	Quartz	Feldspar	Carbonate			
Bohai Bay Basin	1	L69	3043.85	90	4.80	440	1.76	14.43	13	16	2	66	33	2.60	6.69
	2	L69	3048.85	90	2.22	433	5.22	13.76	6	9	1	82	33	1.75	4.21
	3	L69	3045.85	60	2.39	442	1.24	10.78	16	16	1	63	32	2.63	6.99
	4	L69	3045.85	90	2.39	442	1.24	10.78	16	16	1	63	32	2.00	4.98
	5	L69	3050.35	60	5.18	443	2.35	18.56	16	17	2	61	32	3.11	5.79
	6	L69	3050.35	90	5.18	443	2.35	18.56	16	17	2	61	32	1.72	4.77
	7	S352	3183.10	80	5.23	443	0.67	8.47	54	22	7	14	17	2.40	1.77
	8	S352	3183.10	100	5.23	443	0.67	8.47	54	22	7	14	17	2.06	1.93
	9	S352	3183.10	120	5.23	443	0.67	8.47	54	22	7	14	17	1.99	1.98
Songliao Basin	10	Y15	2166.88	90	2.49	428	2.29	7.64	34	31	27	6	10	2.74	3.00
	11	G271	1834.41	90	5.08	450	1.79	26.97	28	32	18	18	14	3.62	2.50
	12	Y15	2180.02	60	1.63	412	1.65	5.59	27	35	24	11	13	3.01	3.46
	13	Y15	2180.02	90	1.63	412	1.65	5.59	27	35	24	11	13	1.37	0.97
	14	G271	1836.41	60	1.73	446	0.51	9.21	31	32	15	19	14	2.95	2.27
	15	G271	1836.41	90	1.73	446	0.51	9.21	31	32	15	19	14	1.63	0.76
Orodos Basin	16	YY33-2	1609.40	30	5.15	445	6.88	12.55	51	22	14	13	22	6.14	1.43
	17	YY33-2	1609.40	40	5.15	445	6.88	12.55	51	22	14	13	22	5.74	1.49
	18	YY33-2	1609.40	50	5.15	445	6.88	12.55	51	22	14	13	22	5.23	2.12
	19	YY33-2	1609.40	60	5.15	445	6.88	12.55	51	22	14	13	22	4.52	2.68
	20	YY33-2	1609.40	70	5.15	445	6.88	12.55	51	22	14	13	22	4.15	2.89
	21	YY34-1	1392.19	30	4.76	443	6.76	11.35	48	24	17	11	25	5.83	1.42
	22	YY34-1	1392.19	40	4.76	443	6.76	11.35	48	24	17	11	25	5.23	1.48
	23	YY34-1	1392.19	50	4.76	443	6.76	11.35	48	24	17	11	25	3.99	1.71
	24	YY34-1	1392.19	60	4.76	443	6.76	11.35	48	24	17	11	25	3.16	2.06
	25	YY34-1	1392.19	70	4.76	443	6.76	11.35	48	24	17	11	25	2.83	2.21
	26	YY21-2	1603.73	60	3.28	434	3.86	8.67	57	19	10	14	19	4.01	4.38
	27	YY8-6	1603.12	60	0.91	478	0.21	0.47	51	44	5	0	16	2.12	2.88
	28	YY26-3	1501.85	57	4.05	437	5.86	9.56	51	26	16	7	20	3.77	2.92
	29	YY9-3	1671.32	62	5.29	457	5.30	8.28	55	32	10	3	22	5.68	3.00
	30	YY12-2	1753.25	64	6.11	458	2.97	6.26	41	30	14	15	27	5.47	2.35
	31	YY13-9	1360.08	53	6.01	454	3.89	10.78	43	42	10	5	40	6.35	3.45
	32	FY2-3	1409.00	54	1.11	460	0.90	1.04	36	33	20	11	18	2.59	3.70