PETROLEUM SCIENCE AND TECHNOLOGY
2016, VOL. 34, NOS. 11–12, 1008–1015
http://dx.doi.org/10.1080/10916466.2016.1176042

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Assessing shale gas resources of Wufeng-Longmaxi shale (O3w-S1l) in Jiaoshiba area, SE Sichuan (China) using Petromod II: Gas generation and adsorption

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ABSTRACT
Taking Well JY4 as example, the authors present petroleum system modeling with PetroMod software for shale gas resource assessment of Wufeng-Longmaxi shale in Jiaoshiba area, which takes account of hydrocarbon adsorption process within source rocks. On the basis of burial and thermal modeling, source rocks adsorption parameters obtained from isothermal adsorption of gas measurements were defined. The results show that the total gas content of Wufeng-Longmaxi shale is estimated in rang of 4.6–10.5 $* 10^6$ kg/km^2, and the proportion of absorbed gas content is around 22–50% in Jiaoshiba area.

KEYWORDS
Gas adsorption; gas generation; Jiaoshiba area; shale gas; Sichuan basin; Wufeng-Longmaxi shale

1. Introduction

Shale gas refers to the natural gas stored in interior of shale rock, which is a typical *in situ* reservoir. The resources assessment of shale gas is a key problem in exploration of unconventional gases (Pollastro, 2007; Jarvie, 2012; Romero-Sarmiento et al., 2013). Majority of shale gas is in free and adsorbed state, and the statistical proportion of adsorbed gas is generally ranging from 20% to 80% (Pollastro, 2007; Jarvie, 2012; Romero-Sarmiento et al., 2013). In a conventional gas reservoir, the adsorption gas content is low (generally less than 20%), which plays a negligible role in the gas reserves. So, routine gas resources assessment need not take account of gas adsorbed process (Pollastro, 2007; Romero-Sarmiento et al., 2013). However, most numerical models and analytical techniques were initially designed for conventional resources. For unconventional gas resources estimation, the assessed gas resources will be less than the actual one without considering adsorbed gas. Nowadays, petroleum system modeling provides an important alternative to evaluate the oil and gas content retained within source rocks, which can be used for unconventional gas resources assessment (Bryant et al., 2013; Romero-Sarmiento et al., 2013).

The Paleozoic strata in Sichuan Basin (China) have attracted a widespread attention in recent years due to its huge shale gas resources (Guo and Zhang, 2014; Guo et al., 2014). Jiaoshiba is an important target for its successful exploration in shale gas. Late Ordovician to early SilurianWufeng-Longmaxi shale (O3w-S1l) is regarded as good source and reservoir rocks due to its good thickness and high organic matter content (Guo and Zhang, 2014; Guo et al., 2014). In this study, we reconstructed the hydrocarbon generation and adsorption histories of Wufeng-Longmaxi shale of Well JY4, analyzed its gas content of total generation and adsorption. These results were subsequently used for assessing shale gas resources in this area. The modeling was built on the burial and thermal histories, which we discussed in Part I of this

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Table 1. Source rock geochemical characteristic of Wufeng-Longmaxi shale in JY4.

Well	Formation	Depth, m	Kerogen type	T_{max}, °C	TOC, %	VR_r, %
JY4	S1l	2494–2551	II	445–522	1.0–2.6	2.2
JY4	S1l	2555–2592	II	446–526	2.6–3.3	2.3
JY4	O3w	2593–2598	I	446–532	4.6–6.5	2.5

series. The whole study was completed by using petroleum system modeling technique with PetroMod software.

2. Hydrocarbon generation model and calibration

Here, we chose Wufeng-Longmaxi shale of Well JY4 to simulate the hydrocarbon generation history. The source rock geochemical parameters required will be discussed in detail subsequently.

2.1. Source rock geochemical characteristics

The geochemical characteristics of Wufeng-Longmaxi shale of Well JY4 include total organic carbon (TOC), organic matter type, hydrogen index (HI), temperature of maximum pyrolysis yield (T_{max}), vitrinite reflectance (VR_o), and thickness of effective source rock are analyzed through the technical report and published papers (Table 1). The TOC content of the shale ranges from 1.0% to 6.5% and organic matter type is mainly sapropel-humic one (Type II). The HI values are between 250 and 600 mg HC/g TOC. The vitrinite reflectance and T_{max} values of Wufeng-Longmaxi shale ranges from 2.2% to 2.5% and 446 to 522°C, respectively, indicating an overmaturated stages. The thickness with rich organic matters (TOC >1.0%) is about 84 m. These geochemical data show that Wufeng-Longmaxi shale is good source rock with great hydrocarbon generation potentials (Guo et al., 2014; Yan et al., 2015).

2.2. Hydrocarbon generation kinetics

Hydrocarbon generation kinetics has been widely used to study hydrocarbon generation history of the source rocks (Burnham and Sweeney, 1989). The Wufeng-Longmaxi shale rocks show high level of maturities, therefore it is hard to find a suitable sample with lower maturity to conduct thermal simulation experiments in and retrieve kinetic parameters of hydrocarbon generation. Previous studies show the kinetic parameters are relatively similar when the organic matter type and lithologies of source rocks are similar (Gao and Hao, 1998; Wang et al., 2005). So, it is reasonable using the published hydrocarbons generation kinetics of similar source rocks with similar kerogen type and lithologies for Wufeng-Longmaxi shale (Pepper and Corvi, 1995; Tomić et al., 1995). Here, we compared three published kinetic parameters by constraining transformation rate (TR) of the generation of C1-C5 gases with actual ones to obtain the most suitable kinetic parameters, which are Type II kerogen of Pepper's model and Type II kerogen of Tang's model provided by PetroMod, and widely used Type II kerogen of Xiahuayuan shale (the upper Proterozoic marine shale in North China).

As shown in Figure 1, the modeled TR of C1-C5 gases by using three kinetic parameters are quite different. The highest is the results from Pepper's Type II model, the middle one is the result from Tang's Type II model and the results from Type II model of Xiahuayuan shale are much lower. We also compared the modeled TR of C1-C5 gases from three models with measured Type II models derived from laboratory pyrolysis, which is commonly used by industry explorations in Sichuan Basin. From Figure 2, it is found that the modeled TR of C1-C5 gases from Tang's TypeIIshow a higher fitness with the measured results. Therefore, the hydrocarbon generation kinetics of Tang's Type II model was used in this study.

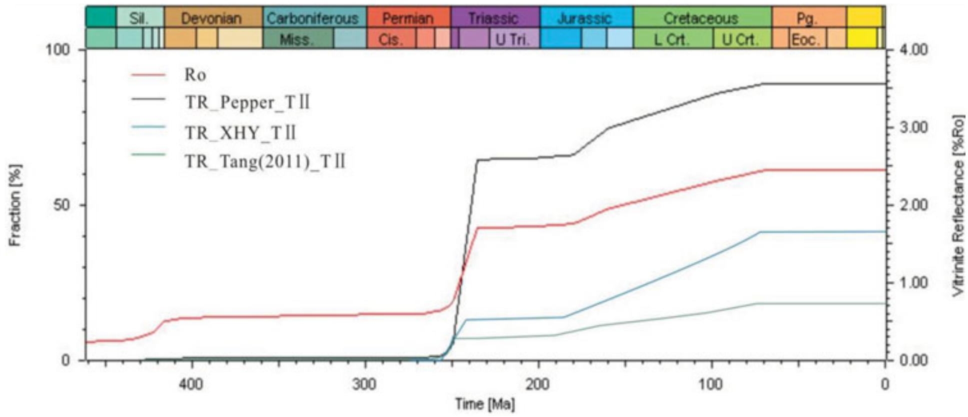

Figure 1. Hydrocarbon generation characteristic of Wufeng-Longmaxi source rock using different kinetics of kerogen.

3. Hydrocarbon adsorption model

3.1. Isothermal methane-adsorbing experiment

Building the hydrocarbon adsorption model should be based on available sorption capacity experiments (Pollastro, 2007; Romero-Sarmiento et al., 2013). It turns out that the maximum adsorption of gases obtained from isothermal adsorption experiments is almost similar to adsorption capacity of shale under the same condition (Pollastro, 2007; Romero-Sarmiento et al., 2013). In this study, two samples (a, b) from Wufeng-Longmaxi shale with different TOC content were selected to conduct the isothermal adsorption experiments under 70°C temperature (Figure 3). TOC value of sample a from the upper part of the shale is 3.09% and TOC value of sample b from the lower part of the shale is as higher as 5.60%. The experiment results show that the maximum adsorption capacity is between 2.75 and 3.0 M^3/ton for upper Wufeng-Longmaxi shale and between 4.25 and 4.5 M^3/t for the Lower Wufeng-Longmaxi shale (Figure 3). TOC content and the pressure are the important factors to control the adsorption capacity of shale. The laboratory data is greatly significant for building the hydrocarbon adsorption model in PetroMod software.

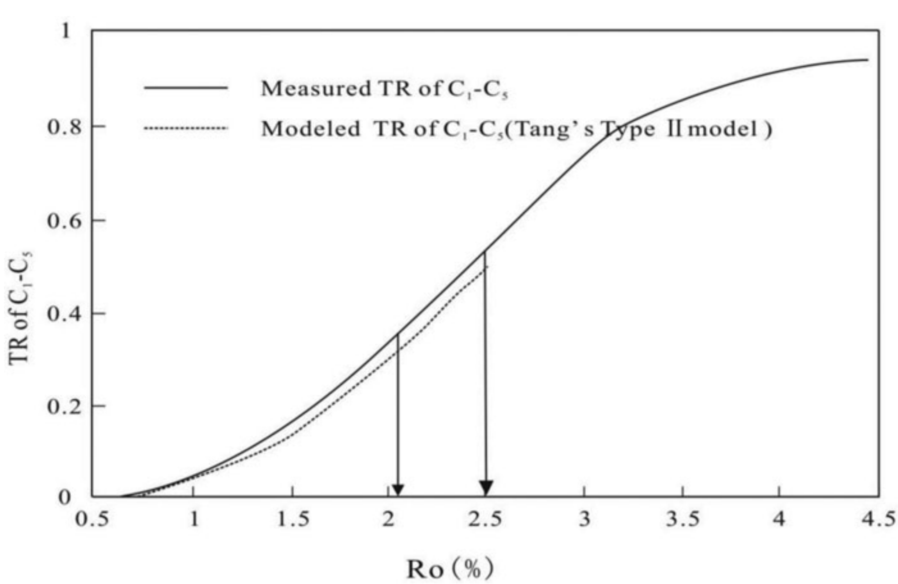

Figure 2. Comparison result of modeled TR (C1-C5) with measured TR (C1-C5).

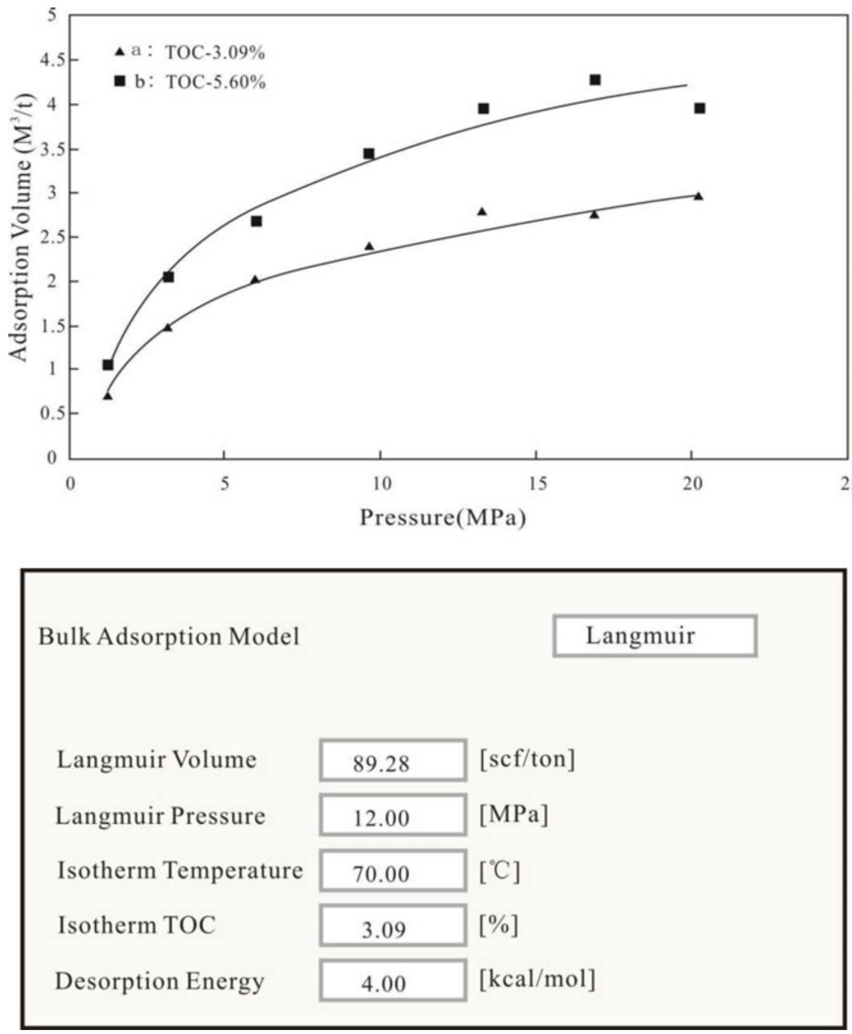

Figure 3. Isothermal adsorption curves (sample a and b) and input parameters of Langmuir adsorption gases model of the Wufeng-Longmaxi shale.

3.2. Hydrocarbon adsorption model within PetroMod

Hydrocarbon adsorption modeling within PetroMod represents a useful alternative to evaluate gas resource retained within shale rock and variations with evolutions of organic matter, temperature and pressure of the rock (Pollastro, 2007; Romero-Sarmiento et al., 2013). Five parameters are needed as input: Langmuir volume (maximum volume of adsorption gas), Langmuir pressure and temperature (laboratory measurement), TOC content, and desorption energy (Figure 3).

4. Results and discussions

4.1. Hydrocarbon generation

Based on the burial and thermal maturity history, the hydrocarbon generation timing of Wufeng-Longmaxi source rock in Well JY4 was discussed in our previous paper (Part I). Here, the hydrocarbon generation potential was defined by calculating the transformation ratio and hydrocarbon yield. As shown in Figure 4, the modeled oil transformation ratio of Wufeng-Longmaxi shale has almost reached 100% in the mid-Triassic, indicating that Wufeng-Longmaxi shale stopped generating oil in that

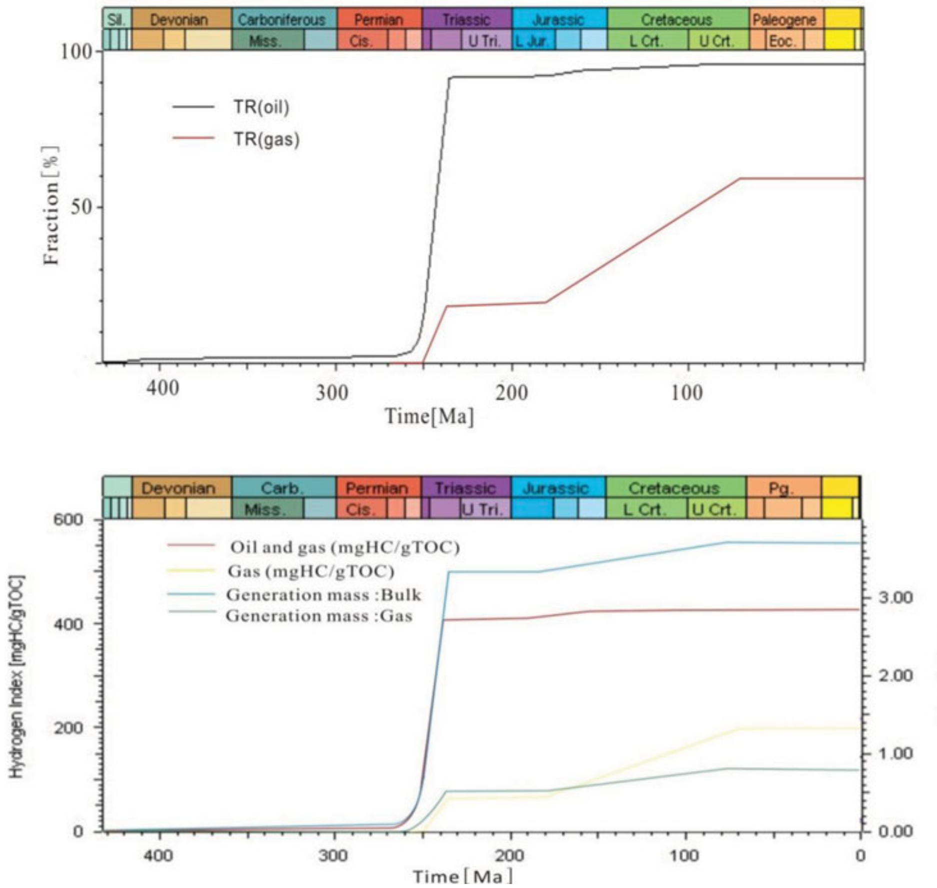

Figure 4. Modeled transformation ratio, hydrocarbon yield and generation mass of oil and gas for the Wufeng-Longmaxi shale.

period. However, at present, the modeled gas transformation ratio just reached 43%, demonstrating the Wufeng-Longmaxi shale is still in the gas generation stage. Tectonic uplift of Himalaya movement prevented it from continually generating hydrocarbon.

After oil generation stopped, the gaseous hydrocarbon began increasing quickly because of cracking of oil. The total hydrocarbon yield ranges from 400 to 429 mL/gTOC, and the gas hydrocarbon yield ranges between 180 and 200 mL/gTOC at present (Figure 4). We calculated that the total petroleum generation intensity reached to almost $4.4 * 10^7$ kg/km^2, and the shale gas generation intensity are about $9.5 * 10^6$ kg/km^2 (gas density is set as 0.7174 kg/Nm^3).

4.2. Hydrocarbon adsorptions

The calculated adsorption capacity of gases for Wufeng-Longmaxi shale of Well JY4 is shown in Figure 5a, indicating that the adsorption capacity changes with pressure and temperature. Pressure and temperature show opposite effects on adsorption equilibrium. Adsorption capacity of shale generally shows a positive correlation with pressure, but a negative correlation with temperature (Romero-Sarmiento, 2013; Yin et al., 2015). From late Cretaceous to present, about 3800 m uplift of O3w-S1l shale leaded to a significant decrease for both pressure and temperature, but the adsorption capacity of the shale show an increasing trend. The main reason is the adsorption capacity of shale shows little changes under high thermal maturity and high pressure state (Yin et al., 2015). After late Cretaceous, the O3w-S1l shale reached a high thermal maturity and pressure (Ro >2.3%, pressure >30 MPa). Based on the previous study on dynamic model of methane adsorption capacity and temperature (Romero-Sarmiento

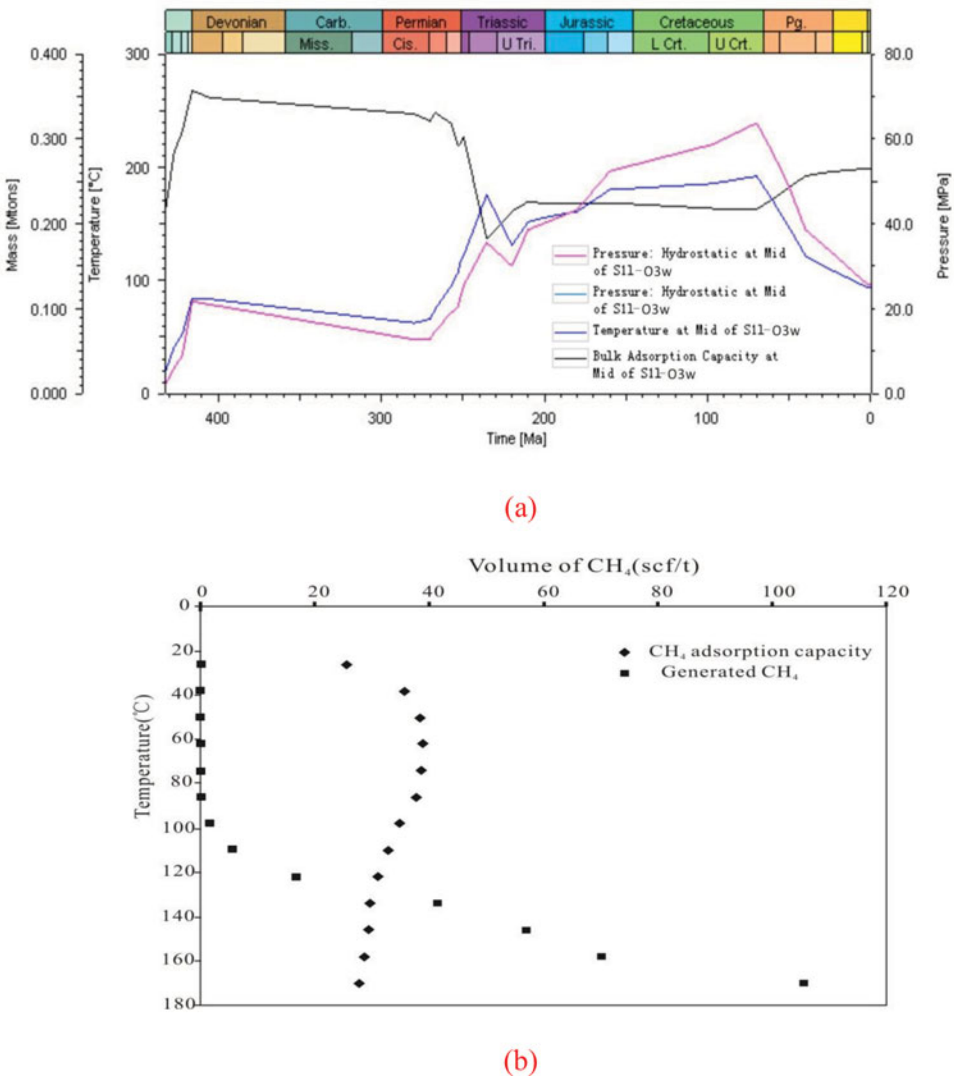

Figure 5. (a) Influence of pressure and temperature on adsorption capacity of Wufeng-Longmaxi shale with Langmuir adsorption model; (b) influence of temperature on CH_4 adsorption capacity and generated CH_4 (Romero-Sarmiento et al., 2013).

et al., 2013), we found that the adsorbed methane would stopping increasing after 60°C, even decreasing slightly with temperature occasionally (Figure 5b). Therefore, the slight increase of adsorption capacity after Late Cretaceous might be caused by a long period of temperature decreasing.

Modeling results also show that in a mature zone of the Wufeng-Longmaxi shale from Well JY4, the total amount of hydrocarbon generation was around $4.4 * 10^7$ kg/km^2 and the amount of generated gas was about $9.5 * 10^6$ kg/km^2 with an average TOC of 3.1% (Figure 6). Applying the Langmuir adsorption model within PetroMod software, the adsorbed gas was estimated about $2.3 * 10^6$ kg/km^2 (approximately 46 scf/t), accounting for more than 24% of the total generated gas. The well-logging results of O3w-S1l source rock in Well JY4 show the total gas content is in the range of 6.0 and 10 m^3/ton and the adsorption gas is between 2.2 and 3.0 m^3/ton. The estimated proportions are about 50–78% free gas versus about 22–50% adsorbed gas, which are consistent with the modeled values. These comparisons indicate that the hydrocarbon generation and adsorption models are relatively reasonable and applicable. Based on these models, we estimated that the total gas of Wufeng-Longmaxi shale was ranging $4.6–10.5 * 10^6$ kg/km^2, and the proportion of absorbed gas was about 22–50% for Jiaoshiba area. However, the model

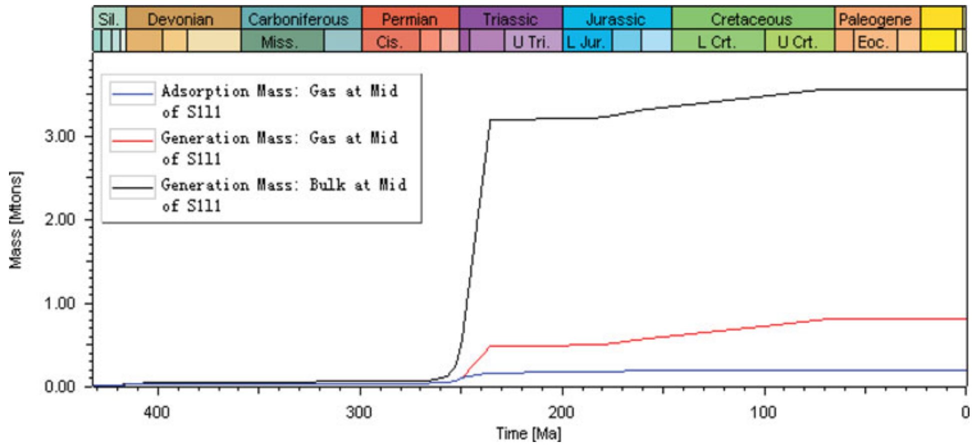

Figure 6. Calculated hydrocarbon resources for Wufeng-Longmaxi shale rock cell of 84 ×1000 × 1000 m with Langmuir adsorption model for gaseous hydrocarbons.

results and the preliminary resources estimations are still need more validating by exploration and well drilling in Sichuan Basin.

5. Conclusions

In this study, we developed a petroleum system modeling with PetroMod software integrating hydrocarbon generation and adsorption processes for shale gas resource assessment. At present day, the Wufeng-Longmaxi shale is still in dry gas generation stage, and its gas transformation ratio is estimated as 43%. Total oil and gas resources in the Jiaoshiba area are around $4.4 * 10^7$kg/km^2 and the gas resources are about $9.5 * 10^6$ kg/km^2.

Adsorption capacity of the Wufeng-Longmaxi shale changes with pressure and temperature, and the change of adsorption capacity after Late Cretaceous was the consequence of long period decreasing of temperature in this area. The modeled adsorption gas is about $2.3 * 10^6$ kg/km^2 for the O3w-S1l shale, and the well-logging results show that the total gas content of Wufeng-Longmaxi shale is about 4.6–10.5 $* 10^6$ kg/km^2 and the proportion of absorbed gas is about 22–50% in Jiaoshiba area.

Funding

The Strategic Priority Research Program of the Chinese Academy of Sciences (XDB10010300), NSFC Project (41372137), CNPC-CAS strategic cooperation project (No. RIPED-2015-JS-255) and GIG 135 project (No.135TP201602) are acknowledged for the financial support. This is contribution No. IS-2247 from GIGCAS.

References

Bryant, I. D., Stabell, C. B., and Neumaier, M. (2013). Evaluation of unconventional resources using a petroleum system modeling approach. *Unconventional Resources Technology Conference*, August 12–14, Denver, CO.

Burnham, A. K., and Sweeney, J. J. (1989). A chemical kinetic model of vitrinite reflectance maturation. *Geochim. Cosmochim. Acta* 53:2649–2657.

Gao, G., and Hao, S. (1998). Hydrocarbon generation dynamics characteristics of kerogen in different source rocks. *Xinjiang Pet. Geol.* 19:372–376.

Guo, T., and Zhang, H. (2014). Formation and enrichment mode of Jiaoshiba shale gas field, Sichuan Basin. *Pet. Explor. Dev.* 41:31–40.

Guo, X. S., Dong-Feng, H. U., Wen, Z. D., and Liu, R. B. (2014). Major factors controlling the accumulation and high productivity in marine shale gas in the lower Paleozoic of Sichuan Basin and its periphery: a case study of the Wufeng-Longmaxi formation of Jiaoshiba area. *China. Geol.* 41:893–901.

Jarvie, D. M. (2012). Shale resource systems for oil and gas: part 1—shale-gas resource systems. *AAPG Memoir* 97:69–87.

Pepper, A. S., and Corvi, P. J. (1995). Simple kinetic models of petroleum formation. Part I: oil and gas generation from kerogen. *Mar. Pet. Geol.* 3:291–319.

Pollastro, R. M. (2007). Total petroleum system assessment of undiscovered resources in the giant Barnett Shale continuous (unconventional) gas accumulation, Fort Worth Basin, Texas. *AAPG Bull.* 91:551–578.

Romero-Sarmiento, M. F., Ducros, M., Carpentier, B., Lorant, F., Cacas, M. C., Pegaz-Fiornet, S., Wolf, S., Rohais, S., and Moretti, I. (2013). Quantitative evaluation of TOC, organic porosity and gas retention distribution in a gas shale play using petroleum system modeling: application to the Mississippian Barnett shale. *Mar. Pet. Geol.* 45:315–330.

Tomić, J., Behar, F., Vandenbroucke, M., and Tang, Y. (1995). Artificial maturation of monterey kerogen (Type II-S) in a closed system and comparison with Type II kerogen: implications on the fate of sulfur. *Org. Geochem.* 23:647–660.

Wang, Y. P., Zhao, C. Y., Wang, Z. Y., Wang, H. J., Zou, Y. R., Liu, J. Z., Zhao, W. Z., Gen, A. S., Liu, D. H., and Lu, J. L. (2005). Kinetic method for determining the main gas-generation period of marine organic matters and its application. *Pet. Explor. Dev.* 32:153–158.

Yan, J. F., Men, Y. P., Sun, Y. Y., Yu, Q., Liu, W., and Zhang, H. Q. (2015). Geochemical and geological characteristics of the lower Cambrian shales in the middle-upper Yangtze area of south china and their implication for the shale gas exploration. *Mar. Pet. Geol.* 70:1–13.