Hydrocarbon generation from confined pyrolysis of Xujiahe Formation coal in the northwest Sichuan Basin, China

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Abstract. The northwest depression of Sichuan Basin is an important gas-producing region. Previous studies have shown that large amount of gas was discovered in the Xujiahe Formaion. Several sets of source rocks from different formations including Xu1, Xu3 and Xu5 sections in Xujiahe Formation contribute to the gas resources. To investigate the gas generation potential of coal measure source rocks of Xujiahe Formation widely distributed in the Sichuan Basin. A coal sample from Xujiahe Formation was used in confined gold tube pyrolysis experiment and the activation energy and frequency factor of the coal sample were obtained. Based on the kinetic parameters of hydrocarbon generation, collected stratigraphic data, the burial, thermal and gas generation history of two wells in the northwest depression of Sichuan Basin were simulated by using Petromod I. Results showed that the activation energy of the coal sample was distributed in the range of 45-67 kcal/mol (main activation energy peak was58 kcal/mol) and the frequency factor was 4.7×10¹¹s⁻¹. For the two investigated wells, the gas generation started at 169-184 Ma, terminated at about 65 Ma. The well CHQ173 closer to the northwest depression entered the threshold of hydrocarbon generation earlier, was of deeper maximum buried depth and higher maximum thermal maturity and greater gas yield. The amount of expelled gas resulted from the uplift was small in this region. If combined with the tectonic evolution and sealing conditions of the study area, the gas generation history of Xujiahe formation would be of great significance for the exploration of natural gas in this area.

1. Introduction
Sichuan basin is one of the important gas-producing basins in China and the northeast depression is an significant gas-producing region of Sichuan Basin. Except for the Feixianguan Formation from Triassic and Changxing Formation from Permian, source rocks of Xujiahe Formation contribute greatly to the gas exploration potential of Sichuan Basin [1]. Although the sedimentation environment, distribution, burial and thermal history of the source rocks from Xujiahe Formation have been investigated [1-3], the gas generation history and potential were still lack of study. In this work, the kinetic parameters of gas generation of a coal sample from Xujiahe Formation were obtained, combined with the burial and thermal history of representative wells from the northwest depression of Sichuan Basin, the gas
generation and expulsion history were simulated by Petromod. This could provide some basic information for the natural gas exploration and exploitation of northwest depression of Sichuan Basin.

2. Geological background
Located in the east of Sichuan Province, Sichuan Basin is one of the most stable sedimentary basins in China, covering an area of $18 \times 10^4$ km$^2$ [4]. It is a superimposed basin of late foreland basin on top of early stable Craton Marine basin. The formation and evolution of Sichuan basin is a long geological process. Subdivided by the large regional faults formed by multi-stage tectonic evolution [5], the Sichuan Basin can be divided into three blocks: central Sichuan, eastern Sichuan and western Sichuan. On this basis, the basin can be divided into six tectonic units: east district, north district, southwest district, central district, west district, and south district (figure 1) [6-7]. The Upper Triassic Xujiahe Formation studied in this paper was made up of six sections from top to bottom. The first, third and fifth stages are the main source rocks, and the second, fourth and sixth stages are the main reservoirs [8-9].

![Figure 1. The location and main structural elements in Sichuan Basin (Modified after [7])](image)

3. Method and workflow
Petromod was used to reconstruct the burial and thermal history of two wells in the northwest Sichuan basin [10-11]. Parameters including the stratigraphy (lithology, thickness and age), tectonic events (unconformities, erosion and age) and boundary conditions (paleo-water depth, heat flow and sediment-water interface temperature) were needed. Xujiahe Formation is mainly composed of terrestrial clastic rocks with coal interlayer and is divided into six sections from bottom to top, the first, third and fifth sections are mainly black mud shale, while the second, fourth and sixth sections are mainly grey fine sandstone [7-9]. In the late Triassic, influenced by The Indosinian movement, the basin changed from Marine facies to continental facies and formed a foreland basin with northwest Sichuan as the sedimentary center. At this time, the sedimentary thickness of Xujiahe Formation was about 250-3500m [12]. Later, affected by the late Himalayan movement, it was unconformably in contact with the overlying strata at a high Angle. Since Triassic, the heat flow value throughout the basin ranged from 50 to 60 mW/m$^2$ [13-14]. The measured Ro of the source rocks in Xujiahe Formation was used to calibrate the parameters.

The sample selected for the kinetic parameters of gas generation is a coal sample from Xujiahe Formation, with total organic carbon content of 68.88%, Ro of 0.61% and Tmax of 421°C. The coal sample was smashed to pass a 200-mesh sieve. The samples were sealed in gold tubes under the protection of argon. 25-40mg power was introduced into each gold tube. Gold tubes were put into
different autoclaves and placed in the same pyrolytic furnace. After thermal pyrolysis, the gas composition and content were determined by HP6890 gas chromatograph with standard method. Based on the gas content generated at each temperature of two sets of experiments with heating rate of 2°C/h and 20°C/h, the kinetic parameters of gas generation were obtained [15-17].

4. Results and discussion
According to the pyrolysis experiment, the hydrocarbon generation amount of the coal sample increased with pyrolysis temperature, and reached about 200 mg/g when the temperature was close to 600 (Figure 2a). The activation energy of C₁-C₅ of the coal sample ranged from 45 to 67 kcal/mol, the distribution of activation energy was mainly asymmetric peak type, and the main peak of activation energy was 58 kcal/mol. The frequency factor (A) was 4.7*10¹¹ S⁻¹ (figure 2b).

![Figure 2](image-url)

**Figure 2.** Total yield of hydrocarbon gases with increasing pyrolysis temperature (a) and kinetic parameters for the Xujiawe Formation coal (b).

Based on the obtained hydrocarbon generation kinetic parameters, stratigraphic and paleo-geothermal parameters, the C₁–C₅ gas generation history and the gas expulsion ratio of two wells in the northwest depression of Sichuan Basin during uplift was estimated (figure 3) [13-14]. From table 1 and figure 3, it can be seen that well FG1 entered the hydrocarbon generation threshold at 169 Ma and produced natural gas continuously. When Ro reached 2.44% at 65 Ma, the gas generation was terminated and the total gas yield was 123 ml/g. The other well CHQ173 entered the hydrocarbon generation threshold at about 184 Ma and reached the highest thermal maturity of 2.74% at 65 Ma. The total gas yield of well CHQ173 at the maximum burial depth was 142 ml/g, which was relatively larger than that of well FG1. The location of well CHQ 173 was closer to the western depression of Sichuan Bain. This led to the deeper maximum burial depth and earlier gas generation of well CHQ173. In terms of uplift, the overall uplift of the northwest depression of Sichuan Basin was small, 3.4% and 5.2%, respectively.
Table 1. Evaluation of gas generation history and uplift characteristics of source rocks in the northwest depression of Sichuan Basin

| Parameters                              | FG1   | CHQ173 |
|-----------------------------------------|-------|--------|
| Time to start gas production/Ma         | 169   | 184    |
| Time to end gas production/Ma           | 65    | 65     |
| Ro/%                                    | 2.44  | 2.74   |
| Total yield /mg/g                       | 123   | 142    |
| Maximum paleo-temperature/°C            | 197.41| 210.51 |
| Current temperature /°C                 | 147.78| 157.66 |
| Temperature difference/°C               | 49.63 | 52.85  |
| Maximum paleo-hydrostatic pressure /Mpa| 49.26 | 52.24  |
| Current hydrostatic pressure /Mpa       | 42.58 | 44.37  |
| Pressure difference /Mpa                | 6.68  | 8.05   |
| Gas volume at maximum uplift /m³        | 95.49 | 92.23  |
| Gas volume at minimum uplift /m³        | 98.82 | 97.06  |
| Uplift ratio                            | 3.4   | 5.2    |

Figure 3. C₁~C₅ gas generation history of Xujiahe Formation, CHQ 173 well

If the thickness, TOC distribution of the source rocks from Xujiahe were available, the total gas generation potential could be estimated and the gas generation center could be obtained by using the kinetics parameter of gas generation of the coal sample. The gas generation history was of great significance, when combined with the tectonic evolution and sealing conditions of the Xujiahe Formation.

5. Conclusions
The kinetic parameters of the gas generation for a coal sample from Xujiahe Formation was investigated by using the confined gold tube pyrolysis equipment. By combing the kinetics parameters, burial and thermal history, the gas generation and expulsion history of two wells in the northwest depression of Sichuan Basin were simulated by using Petromod I. The following conclusions can be drawn:

(1) The activation energy was distributed in the range of 45-67 kcal/mol and the main peak of activation energy was 58 kcal/mol. The distribution of activation energy was mainly asymmetric peak type. The frequency factor (A) was 4.7*10¹¹ s⁻¹.

(2) The well CHQ173 closer to the western depression entered the threshold of hydrocarbon generation earlier, was of deeper maximum buried depth, higher maximum thermal maturity and greater gas yield. The overall uplift of the northwest depression of Sichuan Basin was small and the amount of gas expulsion resulted from the uplift was also small.

The gas generation history of Xujiahe formation would be of great significance for the exploration of
natural gas in this area, when combined with the tectonic evolution and sealing conditions of the Xujiahe Formation.

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