Contents lists available at ScienceDirect

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Material composition, pore structure and adsorption capacity of low-rank coals around the first coalification jump: A case of eastern Junggar Basin, China

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ARTICLE INFO

Keywords: Coalification jump Material composition Pore structure Adsorption capacity Low-rank coal Eastern Junggar Basin

ABSTRACT

The first coalification jump (FCJ) has a significant impact on low-rank coal reservoir heterogeneity, and is of great importance for coalbed methane (CBM) development. Here, a series of experiments were performed for 10 coal samples collected from eastern Junggar Basin, to compare the material composition, pore structure and adsorption capacity of lignite and candle coal. Contrast with the candle coal, the lignite has a higher inertinite content, larger pore volume, better connectivity, and greater specific surface area (SSA). During the process of FCJ, the polycondensation of coal molecules and the compaction of coal matrix occur, leading to a rapid decline of moisture, porosity and permeability, and the cell wall in the candle coal is badly crushed with clay minerals filled from optical microscopy. In general, the larger total pore volume (1.7–300 nm, measured by N_2 adsorption) contributes to the larger SSA. The SSA of candle coal mainly comes from the contribution of micropore (< 10 nm), especially the 2–3 nm pores, while the micropore and transition pore (10–100 nm) contribute to most of SSA of lignite. However, though the SSA of the candle coal is largely lower than that of the lignite, the CH₄ adsorption capacity tends to decrease from the lignite to the candle coal due to material composition difference. Low-field NMR was used to determine the pore and fracture system by analyzing the transverse relaxation time, which showed that only two obvious peaks could be identified in lignite and three peaks at about 0.25 ms, 30 ms and 200 ms are present in the candle coal. The fractal results indicate that the pore surface and complexity inside the coal increase gradually from lignite to candle coal. These observations could deepen awareness and understanding of low-rank coal reservoir heterogeneity and the influence of FCJ on reservoir property.

1. Introduction

The development of coalification is not a straight line but a few jumps because of the physicochemical changes of coal components [1]. This process of evolution is called the coalification jump. Being the key geological event in the coal metamorphism of coal, the coalification jump greatly affects the material composition and molecular structure of coals. Moreover, it controls the physical properties of coal reservoirs, such as the pore volume, surface area, CH₄ adsorption ability, etc. [2,3]. The first coalification jump (FCJ) is characterized by the occurrence of bituminization. As the coal rank increases, enriched-oxygen functional groups gradually fall off. When the maximum vitrinite reflectance ($R_{o,m}$) is less than 0.5%, the products are mainly CO₂ and H₂O. However, when $R_{o,m}$ reaches 0.5–0.6%, as the aliphatic functional groups

and side chains begin to peel off the aromatic fused rings, the CH_4 dominated volatiles are formed [4,5]. Therefore, the FCJ is regarded as the critical geological transition from lignite to bitumite, which usually occurs at $R_{o,m}$ of 0.5–0.6% [4–7]. The coal shape and its physical, chemical, geochemical and petrological properties vary greatly before and after the jump. The earliest exploration on the FCJ could be traced back to late 20th century, which focused on the changes in material composition and interior structure in coals caused by the jump [6–9]. Nevertheless, the heterogeneity features of the development of multiscale pore-fracture in low-rank coal reservoirs around the FCJ are rarely studied in literature.

In the current study, ten coal samples collected from eastern Junggar Basin with R_o in the range of 0.41–0.67% were analyzed using a variety of techniques to reveal the characteristics of material

http://dx.doi.org/10.1016/j.fuel.2017.09.087





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Received 22 July 2017; Received in revised form 9 September 2017; Accepted 21 September 2017 0016-2361/@ 2017 Elsevier Ltd. All rights reserved.

composition (including macerals, ash, moisture, volatile and major elements) and pore-fracture properties (including pore size, shape, structure, type, specific surface area (SSA) and fractal characteristics) of low-rank coals around the FCJ. Furthermore, the effect of FCJ on the adsorption capacity of coal was discussed. This study is important to comprehensively and systematically reveal the material composition and pore size distribution in low-rank coals from a microscopic perspective, and it also has practical significance for CBM exploration and exploitation from low-rank coal reservoirs.

2. Geological setting and analytical procedures

2.1. Geological setting

The Junggar Basin is located in the northern Xinjiang Uygur Autonomous Region, north-west of China, and it is the second largest inland basin in China. The basin covers an area of 13×10^4 km² with 370 km from north to south and 700 km from east to west. The study area is situated in the east of Junggar Basin and is composed of fifteen secondary structural units. The eastern Junggar region was strongly transformed by Late Indosinian movement, which further enhanced the chessboard-shaped structural framework with uplifts and depressions alternation. The seismic reflection formation below Cretaceous of this area has a chessboard-shaped structural framework with convex and concave alternation and picturesque disorder (Fig. 1). The tectonic uplift of Kelameili Mountain provides the source of the Jurassic for the eastern Junggar region. Large-scale continental coal-forming lacustrine in Yanshanian period made Badaowan formation (J₁b) deposition have filling up characteristics where only locally develop minable coal seam.

During the deposition of the Xishan formation (J_2x) where most of the main coal seams occur, the basin was in a balanced subsidence stage. The tectonic evolution and sedimentary characteristics control the coal seam development characteristics. Therefore, Badaowan formation of Lower Jurassic (J_1b) and Xishanyao formation of middle Jurassic (J_2x) are two main coal-bearing strata, which are widely distributed in the basin. Besides, most of the coal in the eastern Junggar Basin is typical and favorable low-rank coal with R_o of 0.38–0.7%. In order to reveal the differences in material composition, pore-fracture system and characteristics of the adsorption capacity of low-rank coals around the FCJ, ten fresh coal samples from Xishanyao Formation in different mining areas (Fig. 1) were collected and analyzed.

2.2. Analytical procedures

2.2.1. Material composition

Firstly, coal samples were analyzed for proximate analysis under air dried basis following the Chinese national standard GB/T 212-2008[10]. According to ISO 7404.3-1994 [11] and ISO 7404.5-1994 [12], mean vitrinite reflectance (R_o) measurements and maceral analyses (500 points) were performed on the same polished section of the coal samples using a Leitz MPV-3 photometer microscope. The X-ray fluorescence spectroscopy (XRF) was used to determine the oxides of major elements, including SiO₂, Al₂O₃, CaO, K₂O, Na₂O, Fe₂O₃, MnO, MgO, TiO₂, and P₂O₅, following the method described in Ryu et al. (2011) [13].

2.2.2. Pore structure

Based on the material composition analysis results, eight samples



Fig. 1. Geographical position of the tectonic units, along with the stratigraphic column for the coal-bearing strata in eastern Junggar Basin.

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