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Quantitative model for predicting the desorption energy of water contained in lignite

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ABSTRACT

Due to the high moisture content (25–65%) dewatering is essential for the clean and efficient utilization of lignite as fuel or feedstock for chemical industry. In order to quantitatively evaluate the desorption energy of contained water content, a prediction model was proposed in this paper based on Lennard-Jones 10-4-3 solid–fluid potential equation and Clausius–Clapeyron principle using lignite pore structure and specific surface area. Based on the proposed model, the drying behavior of two typical Chinese lignite respectively collected from coal mine at Xinjiang and Inner Mongolia districts were experimentally studied and intelligent gravimetric analysis (IGA) was employed for model evaluation. Results show that the water content of original coal sample are 22.4% and 37.6% by weight for Xinjiang and Inner Mongolia lignite, respectively. After air drying at 40 °C, the water content can be dramatically reduced to 13.4% and 17.9%. The overall dewatering energy of the retained moisture after air dying are 38.84 kJ/(100 g air dried coal) for Xinjiang lignite and 53.57 kJ/(100 g air dried coal) for Inner Mongolia lignite. From IGA analysis, it was found that the gradient of the desorption energy of Xinjiang lignite against water content can be separated into three main water desorption stages according to the energy cost.

1. Introduction

Most coal is presently burned as pulverized powder in large-scale furnaces for generating electric power or heat [1]. About 45% of the world coal reserve is lignite which is brownish black in color and has relative high content of volatile matter making it very suitable for chemical utilization such gasification or liquefaction [2]. Unfortunately, lignite also contains very high moisture content which significantly reduces its heating value and makes it very susceptible to spontaneous combustion. When lignite is directly used as fuel in furnace, 20–25% of the calorific value is wasted for converting the inherent water into vapor which may strongly increase the corrosion risk of heat exchanger units [3–5]. So dewatering is considered as an essential pretreatment process and it has been reported [6] that only by reducing the coal moisture for 5%, the overall boiler efficiency can approximately increase 2.6%. Moreover, under the same boiler output load, the fuel flow rate and flue gas volume can respectively reduce 10.8% and 4%. Although dewatering pretreatment can achieve many economic and environmental benefits, it consumes extra energy or chemical material and previous research has found that the characteristics of water content and their interaction with the coal surface will strongly affect the dewatering energy cost [7–12].

In the past few years, many methods have been developed for characterizing the moisture adsorbed in lignite. According to the energy required for water desorption, Allardice and Evans [13] suggested that at any particular temperature there were at least two types of water existing in Yallourn brown coal including water which can be removed by evacuation and water which can be released only by raising the temperature. From distinct forms of moisture contained in coals, Karr [14] defined five types of water associated within the coal and they respectively are (a) interior adsorption water which is contained in micro pores and micro capillary; (b) surface adsorption water which forms a layer of water molecules adjacent to coal molecules and on the particle surface only; (c) capillary water which is contained in macro capillaries; (d) inter particle water which is contained in small crevices found between two or more particles; and (e) adhesion water which forms a layer or film around the surface of individual or agglomerated particles. Based on the congelation properties, Norinaga et al. [15] declared three types of water adsorbed in coal including free water, bound water and non-freezable water that never freezes at any given temperature. The contents of the free and bound waters were experimentally determined from the congelation heat, and then the non-freezable water could be calculated by the difference.

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Currently, the most widely studied lignite dewatering method includes mechanical, thermal and chemical drying [5]. Thermal drying is considered as the most commercialized technology for industrial utilization except for the high energy consumption. During thermal drying, the coal particles are directly or indirectly heated up to the desired temperature at which the contained water can overcome the interaction with coal particle and evaporate. Although many different thermal drying technologies have been developed and some of these technology have already been widely used [5], there still lacks fundamental model to quantitative describe the detailed energy consumption due to the complex of the interaction between different kinds of water with coal particle.

In this paper, a mathematical model was proposed based on the Lennard-Jones 10-4-3 solid–fluid potential equation and the Clausius–Clapeyron equation to calculate the detailed energy of water in typical lignite from the study of adsorption of moisture on single solid surfaces and in micro pores [16]. The sorption/desorption isotherms were used to deduce the specific surface area and moisture losing rate during desorption through intelligent gravimetric analysis (IGA) under different pressure. Two kinds of typical Chinese lignite were experimentally studied and the results can be used for predicting water evaporation energy cost and for optimizing the thermal dewatering system.

2. Water desorption energy calculation model

According to the interaction between the moisture and the coal surface, the water can be classified into crystal water, molecular water and capillary water. These different water are constrained in the different micro geometric location of the coal. Fig. 1 shows the microstructure of the Xinjiang lignite sample used in this paper along with the existence model of contained water proposed in previous study [17]. When the lignite is heated during thermal drying, the energy required for water evaporation can be divided into four parts including (a) the energy for water droplets to overcome the chemical bounding; (b) the energy for overcoming the intermolecular physical interaction; (c) the energy for overcoming the capillary force, and (d) the energy for water phase changing. The chemical desorption energy is used to break the chemical bound between the coal chemical species (mostly metal salts) and the crystalized water molecule. According to previous study [18], it is very difficult to remove this part of water by traditional thermal drying method, because water is firmly bonded to the coal surface [19]. So in this paper, to simplify the calculation, a previous measured constant value (Q_1) is assumed to indicate the energy to overcome the chemical bounding force. The physical desorption energy is defined as the energy for breaking the physical interaction between the coal particle and the molecular water. Allardice and Evans [20] studied the drying behavior of Yallourn brown coal containing 196 g of water per 100 g dry coal. They observed that below water contents of 15 g per 100 g dry coal, the desorption heat increases steeply and suggested that the increase can be attributed to the changing from multilayer water evaporation to monolayer water evaporation and the monolayer water is strongly bounded to coal surface. According to surface physical chemistry mechanism [21] and molecular thermodynamics, the interaction between a solid surface molecule and a water molecule includes Keesom force, Debye force, London dispersion force and repulsive force [22]. The energy required to overcome these forces are proportional with the distance between the molecule of coal species

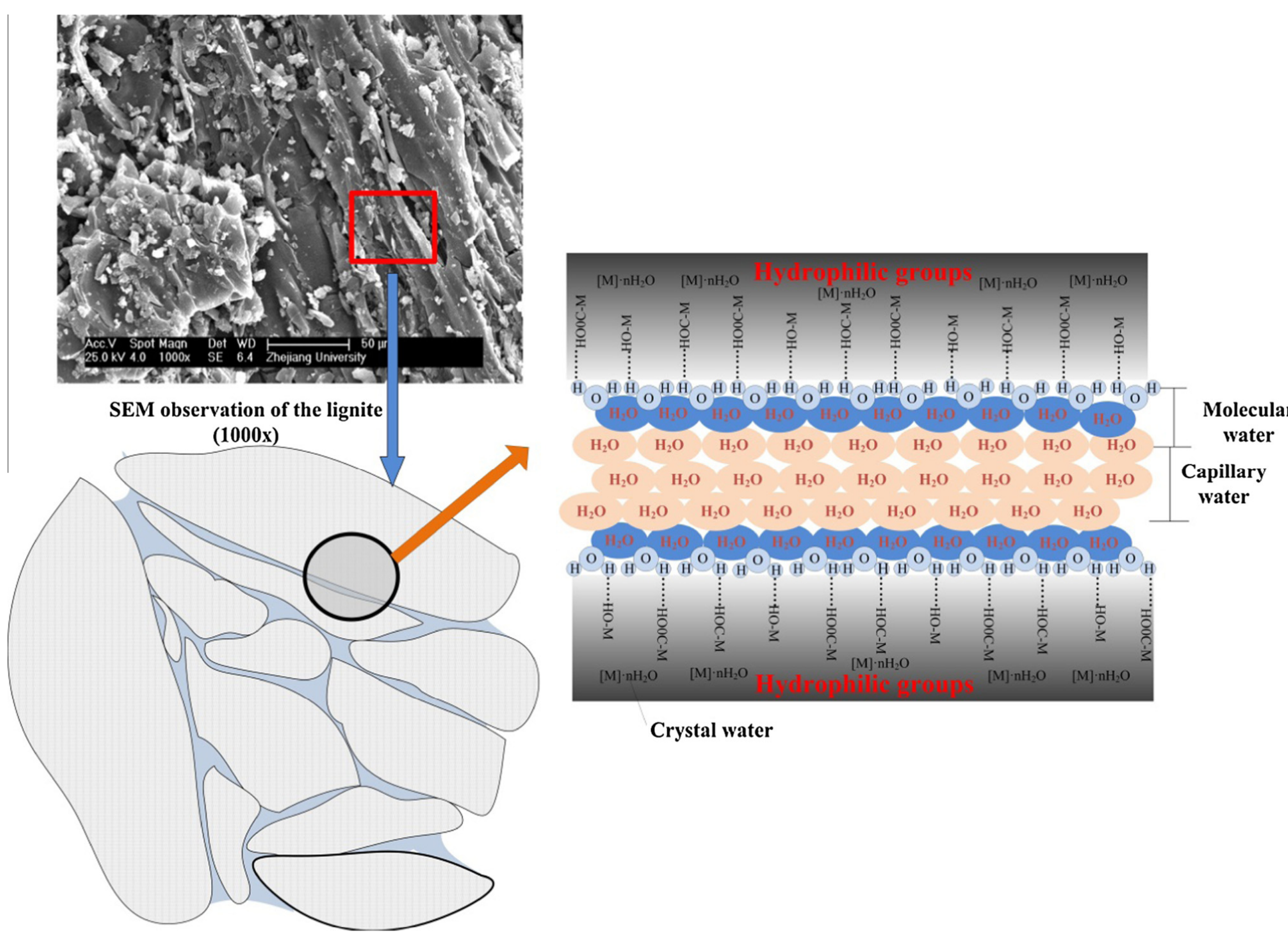

Fig. 1. Microstructure of moistened lignite [17].