

Accepted Manuscript

Construction of a macromolecular structural model of Chinese lignite and analysis of its low-temperature oxidation behaviour

Xianliang Meng, Mingqiang Gao, Ruizhi Chu, Zhenyong Miao, Guoguang Wu, Lei Bai, Peng Liu, Yuanfang Yan, Pengcheng Zhang

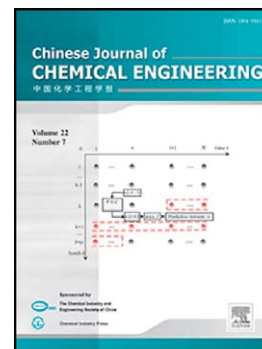
PII: S1004-9541(17)30585-2
DOI: doi:[10.1016/j.cjche.2017.07.009](https://doi.org/10.1016/j.cjche.2017.07.009)
Reference: CJCHE 883

To appear in:

Received date: 15 May 2017
Revised date: 8 July 2017
Accepted date: 10 July 2017

Please cite this article as: Xianliang Meng, Mingqiang Gao, Ruizhi Chu, Zhenyong Miao, Guoguang Wu, Lei Bai, Peng Liu, Yuanfang Yan, Pengcheng Zhang, Construction of a macromolecular structural model of Chinese lignite and analysis of its low-temperature oxidation behaviour, (2017), doi:[10.1016/j.cjche.2017.07.009](https://doi.org/10.1016/j.cjche.2017.07.009)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Energy, Resources and Environmental Technology**Construction of a macromolecular structural model of Chinese lignite and analysis of its low-temperature oxidation behaviour[☆]**

Xianliang Meng^{a, b}, Mingqiang Gao^b, Ruizhi Chu^{a, b*}, Zhenyong Miao^b, Guoguang Wu^b, Lei Bai^c, Peng Liu^b, Yuanfang Yan^b, Pengcheng Zhang^b

^a Key Laboratory of Coal-based CO₂ Capture and Geological Storage, Jiangsu Province (China University of Mining & Technology), Xuzhou 221116, China

^b School of Chemical Engineering and Technology, China University of Mining & Technology, Xuzhou 221116, China

^c Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown 26506, the United States of America

Abstract: The aim of this paper is to analyze the change in the active structure of lignite during the process of low-temperature oxidation by constructing a molecular structure model for lignite. Using quantum computation combined with experimental results of proximate analysis, ultimate analysis, Fourier transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS), a structural model for the large molecular structure was constructed. By analyzing the bond lengths in the model molecule, the evolution law for the active structure of lignite was predicted for the process of low-temperature oxidation. In low-temperature oxidation, alkanes and hydroxyls are the primary active structures observed in lignite, though ether may also react. These active functional groups react with oxygen to release heat, thereby speeding up the reaction between coal and oxygen. Finally, the content of various functional groups in the process of lignite low-temperature oxidation was analyzed by infrared analysis, and the accuracy of the model was verified.

Keywords: Chinese lignite, coal combustion, molecular simulation, low-temperature oxidation process, environment

[☆] Supported by the Fundamental Research Funds for the Central Universities (2017XKQY066).

* To whom correspondence should be addressed.

E-mail: ruizhichu@126.com

Download English Version:

<https://daneshyari.com/en/article/4764048>

Download Persian Version:

<https://daneshyari.com/article/4764048>

[Daneshyari.com](https://daneshyari.com)