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PII: S1004-9541(17)30685-7
DOI: doi:10.1016/j.cjche.2017.09.021
Reference: CJCHE 938

To appear in:

Received date: 3 June 2017
Revised date: 14 September 2017
Accepted date: 22 September 2017

Please cite this article as: Guodong Wang, Jianchun Jiang, Kang Sun, Jianzhong Wu, An improved theoretical procedure for the pore-size analysis of activated carbon by gas adsorption, (2017), doi:10.1016/j.cjche.2017.09.021

Chemical Engineering Thermodynamics

An improved theoretical procedure for the pore-size analysis of activated carbon by gas adsorption*

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ABSTRACT

Amorphous carbon materials play a vital role in adsorbed natural gas (ANG) storage. One of the key issues in more prevalent use of ANG is the limited adsorption capacity, which is primarily determined by the porosity and surface characteristics of porous materials. To identify suitable adsorbents, we need a reliable computational tool for pore characterization and, subsequently, quantitative prediction of the adsorption behavior. Within the framework of adsorption integral equation (AIE), the pore-size distribution (PSD) is sensitive to the adopted theoretical models and numerical algorithms through isotherm fitting. In recent years, the classical density functional theory (DFT) has emerged as a common choice to describe adsorption isotherms for AIE kernel construction. However, rarely considered is the accuracy

* Supported by National Sci-Tech Support Plan (2015BAD21B05) and China Scholarship Council (201408320127).

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