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P. Brea, J.A. Delgado, Vicente I. Águeda, María A. Uguina

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## **ACCEPTED MANUSCRIPT**

# Comparison between MOF UTSA-16 and BPL activated carbon in hydrogen purification by PSA

P. Brea<sup>a</sup>, J.A. Delgado<sup>a</sup>, Vicente I. Águeda<sup>a</sup>, María A. Uguina<sup>a</sup>

<sup>a</sup>Department of Chemical Engineering, Universidad Complutense de Madrid, 28040 Madrid, Spain.

Keywords: Metal-organic framework; activated carbon; PSA; simulation; H<sub>2</sub> purification.

#### **HIGHLIGHTS**

- Laboratory scale PSA hydrogen purification cycle experiments with two adsorbents: BPL AC and UTSA-16.
- Simulations of PSA cycles performed in the experiments with PSASIM®.
- Comparison of UTSA-16 and BPL AC with simulations of a PSA cycle for hydrogen purification.

#### **Abstract**

The aim of this work is to study the application of Metal-Organic Framework (MOF) UTSA-16 in hydrogen purification PSA processes since UTSA-16 can adsorb/desorb CO, CH<sub>4</sub> and specially CO<sub>2</sub> (typical impurities of a SMR off-gas). PSA experiments (Skarstrom type PSA cycles) for hydrogen purification from a typical SMR off-gas mixture (CH<sub>4</sub>, CO and CO<sub>2</sub> as impurities) were carried out using two adsorbents: MOF UTSA-16 and BPL activated carbon (BPL AC). A simulation tool developed at the University Complutense of Madrid, PSASIM®, has been used to simulate the experimental PSA cycles. The model has been validated by reproducing the experimental results. Finally, a PSA cycle with operating conditions of hydrogen purification processes [1] has been simulated with PSASIM® with layered beds, containing UTSA-16/Zeolite 5A and BPL AC/Zeolite 5A. The results obtained from the

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