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Adsorption of Natural Gas Mixtures in Nanoporos Carbon[1] CARLOS WEXLER, IAN CRAWFORD-GOSS, DREW LEMKE, University of Missouri, MICHAEL ROTH, Northern Kentucky University — Natural gas (NG) is promising fuel due to its smaller CO_2 emissions per unit energy compared to other hydrocarbons [1]. Storage via adsorption into carbon nanostructures permits the operation of storage tanks at significantly reduced pressures, resulting in cost savings, added safety and smaller loss of cargo volume. Since NG is mostly comprised of methane (87-99%), other components are often ignored, even though heavier species are likely to adsorb preferentially and possibly result in long-term performance issues [2]. We performed Molecular Dynamics (MD) simulations to understand the behavior of heavier components of NG adsorbed into carbon nanostructures. We focused on mixtures involving methane, ethane and propane. We show that the heavier components have significant preferential adsorption, partially inhibiting the adsorption of methane, and resulting in its saturation at lower pressures. Under room temperature conditions, propane adsorbs quasi irrevesibly, though remaining mobile within the pores. We discuss the diffusion regime of all gases and address methods to remove the adsorbed heavier gases by thermal cycling the tank. References: [1] L. Ortiz, *et al.*, Mat. Res. Exp. **3**, 055011 (2016). [2] M. Golebiowska, *et al.*, Carbon **50**, 225-234.

[1]American Chemical Society Petroleum Research Fund

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