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Adsorption of Natural Gas Containing Propane in Graphene Nanocells Using Molecular Dynamics Simulations[1] IAN CRAWFORD-GOSS, University of Missouri Columbia, MICHAEL ROTH, Northern Kentucky University , CARLOS WEXLER, University of Missouri Columbia — Natural gas (NG) is a promising fuel for vehicular use due to its comparatively small CO2 emissions. Storage via adsorption into carbon nanocells permits the use of storage tanks at reduced pressures, resulting in cost savings, added safety and smaller loss of cargo volume. Since NG is comprised of methane (87-99%), other heavier components are often ignored in studies. We performed Molecular Dynamics simulations to understand the behavior of the heavier components of NG adsorbed into carbon nanocells. Our studies focus on the adsorption of mixtures of methane and either ethane or propane. In this work we show that propane experiences preferential adsorption, partially inhibiting the adsorption of methane, and resulting in saturation at lower pressures. At room temperature, the adsorption of propane is irreversible (vs. methane which reversibly adsorbs/desorbs by pressure swings). Long-term, this would mean that adsorption tanks would gradually see a reduction of storage and performance without further treatment. However, we also observe that propane remains highly mobile within each pore, with a diffusion constant of the same order of magnitude as that of methane. We discuss possible combined thermal/pressure-swing treatments that would desorb heavier molecules.

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