# $CO_2/H_2S$ Affect Nano-Confined Carbon-Bearing Fluids: Evidence of Facilitated Transport

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The interactions of trapped reservoir gases within organic-rich sedimentary rocks have direct relevance to many geoenergy applications. Among the nanoscale properties that play most significant roles in determining the efficiency of such applications are fluid adsorption capacity, oil displacement efficiency, and fluid transport. Employing molecular dynamics simulations, we probe here these properties for gases containing carbon dioxide ($CO_2$) or hydrogen sulfide ($H_2S$) and methane ($CH_4$) interacting with amorphous silica nano-pores filled with benzene. The results show that, at geological temperature and pressure conditions, both $CO_2$ and $H_2S$ are strongly adsorbed in the organic-filled pore, inducing swelling and displacement of benzene. Unexpectedly, $CO_2/H_2S$ adsorption also facilitates $CH_4$ transport through the benzene-filled pore and might swell benzene, leading to the creation of preferential transport pathways. Analysis of adsorption energies and free energy landscapes confirms that shale gas-organic matters-rock interactions at the nano-scale are key factors governing adsorption and transport behaviour of reservoir gases trapped in caprocks.