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A DFT study on the effect of strain on the adsorption of gas in tight gas carbonates

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Tight unconventional reservoirs are characterized by structural complexation and physical properties that influence the ability to recover and estimate the amount of gas in the rock. One of the physical factors is the change of the strain which may affect the gas interaction with the rocks'surface. To study the effect of strain on the gas-surface interaction, density functional theory (DFT) calculations are conducted to find the adsorption energy of the natural gas'components on the tight-gas carbonated reservoirs. Calcite (104) represents the majority of the calcium carbonate reservoirs; thus, it is selected in this work to represent the tight reservoirs. The gases considered in the study are CH4, CO2, C2H6, and N2, and they all show a physiochemical interaction with the surface for all the considered strain values (-3% to 3%), with CO2 showing the highest adsorption affinity. Along with the weak interaction, there is no specific trend for the change of CH4 adsorption with the strain effect. In contrast, the change in adsorption of CO2 and C2H6 showed more pronounced alteration with strain compared to other gases. For instance, by applying tensile strain, a 25% increase in CO2 adsorption energy is obtained depending on the concentration of the gas molecules. The estimation of ultimate recovery (EUR) could be determined from the obtained results by computing the effects of the geomechanical factors on the adsorption of the gas on the surface of the carbonaceous tight gas reservoirs.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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Primary author: Ms ELBASHIER, Elkhansa (Graduate Student)

Co-authors: Prof. HUSSEIN, Ibnelwaleed (Qatar University); Dr CARCHINI, Giuliano (Research Assistant); SAKHAEE-POUR, Ahmad (University of Houston); Dr BERDIYOROV, Golibjon

Presenter: Ms ELBASHIER, Elkhansa (Graduate Student)

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