



Prediction of CO₂ adsorption-induced deformation in shale nanopores

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**S. Bakhshian
S.A. Hosseini**

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**BUREAU OF
ECONOMIC
GEOLOGY**



TEXAS Geosciences
Bureau of Economic Geology
Jackson School of Geosciences
The University of Texas at Austin

Abstract

Understanding of CO₂ adsorption in shale provides significant information about the potential for geological storage of CO₂ in shale formations to mitigate the impact of carbon emissions on the climate. This work focuses on the adsorption behavior of CO₂ in shale with various pore sizes at a wide temperature range including 31.28 °C, 40 °C, 65 °C, and 90 °C and pressures up to 15 MPa through a comprehensive model. Using a thermodynamic approach, we combine lattice density functional theory with finite element formulation to estimate CO₂ adsorption behavior along with its induced strain in shale nanopores. We study the effect of geometric confinement, including pore size and pore geometry, on the excess adsorption and swelling strain of shale under different temperatures. When the model was applied to sorption of CO₂ in Posidonia Shale samples, all reported experimental features of the phenomenon were reproduced. Although the developed model applied to the specific case of CO₂ adsorption-induced swelling in shale, it is also applicable to any problem regarding adsorption of any fluid confined in a porous medium and its triggered swelling strain.

We found that the highly confined geometry of the duct pore, which applies a large attractive surface field to adsorbed layers, leads to a faster, and a higher amount of adsorption compared with that of a slit pore. This effect is more significant in larger pore widths. The results also demonstrate a sharp rise in the adsorption isotherm and swelling strain near the bulk critical point of CO₂. This phenomenon attributes to the highly compressive behavior of CO₂ near its critical point, which leads to a sharp increase in bulk density and, thus, in adsorbed phase density and its resultant swelling strain. The results also denote that total volumetric strain is a function of temperature, pore width, and pore shape. The effect of pore shape and temperature is more prominent for pores with larger sizes.