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The geochemical effects of impurities in the CO2 stream

Mihrin, Dmytro; Mokhtari, Rasoul; Talaei, Ali; Nick, Hamid; Feilberg, Karen Louise

Publication date:
2023

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Mihrin, D., Mokhtari, R., Talaei, A., Nick, H., & Feilberg, K. L. (2023). *CO2 storage in carbonate reservoirs: The geochemical effects of impurities in the CO2 stream*. Abstract from Danish Offshore Technology Conference 2023 , Kolding, Denmark.

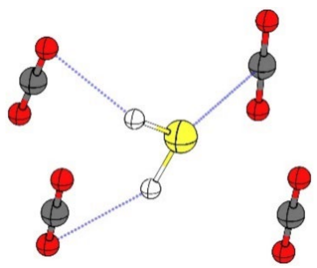
Danish Offshore Technology Centre
Technology Conference 2023

CO2 storage in carbonate reservoirs

The geochemical effects of impurities in the CO2 stream

Dmytro Mihrin, Rasoul Mokhtari, Ali Talaei, Hamid Nick, Karen Louise Felberg

Storage of carbon in the form of compressed CO_2 in the subsurface represents a potentially viable way to reduce emission of heat-trapping CO_2 to the atmosphere. The chemical composition of the CO_2 stream will depend on the fuel sources and capture methods, and CO_2 with impurities is much more widely available. The aim of this study is to consider the effects of CO_2 purity on injectivity and storage in mature chalk and other carbonate subsurface reservoirs in late stages of hydrocarbon production with geological and petrophysical characteristics favourable to CO_2 injection. The nature of these minor impurity constituents in the supercritical CO_2 stream will affect the phase behaviour, viscosity, density, and interfacial behaviour of the CO_2, particularly for the non-compressible impurities N_2, Ar and O_2. Equation of state models based on empirical data exist to model these macroscopic properties, however the models can be greatly improved by measured physical parameters. Phase parameters as well as other chemical and physical properties depend on the intermolecular interactions between the CO_2 molecules and the available impurities, which may for some polar impurities strongly dominate relative to the self-association forces between CO_2 molecules. Using modern theoretical chemistry methodologies (DLPNO-CCSD(T)/MP2) of the molecular interaction strengths between CO_2 itself, chemicals, and reactive surfaces for mitigation of the effects of important impurities such as aminoethanol, ethylene glycol, methanol, ethanol, water, H_2S, NH_3, NO_x, CO and SO_2 are computed employing the high-performance computing (HPC) facilities at DTU. The calculations predict how the impurity molecules are structurally linked to CO_2 and whether the interactions are sufficiently strong to perturb the properties of CO_2 in the pure form significantly (see figure below). The interaction strength of impurities with CO_2, surfaces and other chemicals will indicate how easily effects of different impurities might be mitigated in CO2 sources. These calculations can be used to predict the effect of impurities for which adequate data from field experience are not available, allowing thermodynamical models to be quickly updated. The results are tested in laboratory experiments using carbonate rock samples and impurity doped CO_2 and compared to pure CO_2.



Condensed phase of CO_2 perturbed by H_2S impurity.

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