ICCES, 2024, vol.30, no.2
DOI: 10.32604/icces.2024.011120

PROCEEDINGS

Fast and Accurate Calculation on Competitive Adsorption Behavior in Shale Nanopores by Machine Learning Model

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ABSTRACT

Understanding the competitive adsorption behavior of CO_2 and CH_4 in shale nanopores is crucial for enhancing the recovery of shale gas and sequestration of CO_2, which is determined by both the inherent characteristics of the molecules and external environmental factors such as pore size, temperature, and partial pressures of CO_2 and CH_4. While the competitive adsorption behavior of CO_2/CH_4 has been analyzed by previous studies, a comprehensive understanding from the perspective of molecular kinetic theory and the efficient calculation for competitive adsorption behavior considering various geological situations is still challenging, limited by the huge computation cost of classical molecular dynamics (MD) methods. In this work [1], the theoretical connection between inherent characteristics of molecules and adsorption behavior is firstly built to reveal the general laws in the behavior of CO_2/CH_4 competitive adsorption through posture analysis of the molecules. A machine learning algorithm, aided by molecular kinetic theory, is proposed to facilitate the fast and accurate predictions of competitive adsorption behavior, and detailed analyses of the influencing factors are conducted accordingly. The insights gained from this work provide a foundation for expeditiously optimizing the competitive adsorption behavior of CO_2/CH_4, with potential implications for CO_2 sequestration and enhanced gas recovery (CSEGR) process.

KEYWORDS

CO_2/CH_4 competitive adsorption; shale nanopores; posture analysis; molecular dynamics theory; machine learning algorithms

Funding Statement: This work is jointly supported by the National Natural Science Foundation of China (12202432, 52274058, and U22B2075), the National Postdoctoral Program for Innovative Talents (BX2021285).

Conflicts of Interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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