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Insights into in-situ shale kerogen pyrolysis and gaseous hydrocarbon evolution from ReaxFF molecular dynamics simulation

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This study employs ReaxFF molecular dynamics (ReaxFF-MD) simulations to investigate the hydrocarbon generation mechanisms of typical type II kerogen from the Chang-7 Member of the Triassic Yanchang Formation in the Ordos Basin (NW China) under both isothermal and non-isothermal conditions. The results indicate that during the high-temperature pyrolysis of the Chang-7 shale kerogen, the cleavage of aliphatic side chains and heteroatomic functional groups occurs first, followed by gradual deep depolymerization and aromatization of the carbon skeleton. The generation of light hydrocarbons and inorganic gases exhibits a stage-specific pattern in terms of both time and temperature, with the early stage dominated by loose structural breakdown and limited bond cleavage, while the intermediate and late stages are characterized by deep cracking and molecular miniaturization. Meanwhile, on the basis of non-isothermal thermogravimetric data, the calculated apparent activation energy of kerogen pyrolysis is 51.92 kcal/mol using the Kissinger method, with a good correlation coefficient, validating the reliability of the molecular simulation results.

The composition of gaseous hydrocarbons is highly sensitive to the degree of pyrolysis and can serve as a key indicator for monitoring the in-situ conversion process of shale. Analysis of the evolution of CH_4, C_2H_6, C_3H_8, and C_4H_{10} reveals a clear trend of progressive evolution from higher-carbon-number to lower-carbon-number hydrocarbons as temperature increases. Methane increases monotonically with temperature and accumulates continuously, representing a characteristic product of the deep pyrolysis stage; Ethane reaches a peak in the medium-to-high temperature range before undergoing secondary cracking; while C_3H_8 and C_4H_{10} only exist transiently under relatively low or moderate thermal intensities. This sequence reflects the progression of crude oil and kerogen from primary cracking to deep cracking, providing significant insight for real-time monitoring of the pyrolysis extent during in-situ thermal conversion processes.