Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.28097

Modeling Thermal Cracking of Organic Matter with the Kinetic Monte-Carlo Method

HAO XIE

International Center for Isotope Effect Research, Nanjing University, China

Geochemical investigations of petroleum sources, evolution, and decomposition rely on analyzing the chemical composition and stable isotope ratios of hydrocarbon compounds. Traditional interpretation of these geochemical datasets has primarily depended on empirical relationships derived from field observations or laboratory pyrolysis experiments that simulate thermal cracking. However, due to their empirical nature, these approaches frequently face inconsistencies and ambiguities. A notable example is the existence of multiple conflicting calibration curves for the methane isotope–thermal maturity relationship.

To address these limitations, I developed a reaction model for thermal cracking based on the kinetic Monte Carlo method. The kinetic Monte-Carlo method can solve the master equation of complex reaction systems via stochastic formulation. This model is capable of calculating all molecular species and isotopic forms of products generated from breakdown of macromolecular structures. The embedded chemical kinetic parameters of this model are sourced from quantum chemical calculations, rather than calibrated against empirical datasets. I validated the model against analytical solutions and experimental results of thermal cracking. Application of this model to diverse kerogen structures revealed that carbon isotope variations in methane during early maturation stages are strongly influenced by the enrichment of certain structural groups, such as aromatic-bound alkyl chains. My model establishes a mechanistic link between source materials and their cracking products, offering insights on petroleum generation and thermal evolution of organic matter.