

The effect of pressure on the chemical reaction of an n -C₂₅ alkane under the high-pressure and high-temperature conditions of the interior of the Earth

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Knowledge of the behavior of carbon components in the subducting slab is crucial to understanding the deep carbon cycle. Organic carbon is an important carbon component in the oceanic sediment, and it has been suggested that some amount of organic carbon in the Earth's surface has been subducted into the interior of the Earth beyond the subducting slab. In the subducting slab, both temperature and pressure increase with increasing depth. Higher temperatures enhance thermal cracking with the production of lighter volatiles, whereas pressure induces polymerization with the formation of heavier organics. Thus, the chemical reactions of organics in the subducting slab are expected to be complicated and are currently poorly understood.

Alkanes (C_nH_{2n+2}) are an important part of the organic components of the oceanic sediment. Chemical reactions of alkanes under high-pressure and high-temperature (HPHT) conditions have been investigated previously using diamond anvil cells and spectroscopic analysis. Formation of heavier alkanes and unsaturated carbons from methane (CH₄) and hexane (C₆H₁₄) under HPHT conditions has been reported (Lavanov et al., 2013 and Yang et al., 2021), although the reaction mechanism and kinetics are still unknown because the complex reaction products are difficult to identify individually. In the current study, we investigated the effect of pressure on the chemical reaction of a n -alkane experimentally. Complex reaction products were identified and were evaluated analytically using gas chromatography-mass spectrometry (GC/MS) to reveal the effects of pressure on the reaction process and kinetics.

Pentacosane (n -C₂₅, C₂₅H₅₂) was used as the initial material. Approximately 3 mg of the initial material was mixed with Al₂O₃ and filled in a gold sample capsule. HPHT experiments were performed at 0.5-1.5 GPa and 360-400°C using a piston-cylinder type high-pressure apparatus with a band-type heater. The reaction kinetics were investigated in several experiments by changing the reaction time. The reaction products were recovered to ambient conditions and then analyzed using GC/MS after extracting with a solvent. Insoluble materials were evaluated using Raman spectroscopy.

After heating at 0.5 GPa and 400°C for 48 h, around 10 % of the initial material was recovered, while over 80 % of the initial material was recovered after heating at 1.5 GPa and 400°C for 48 h. The result indicates that the reaction rates decrease with increasing pressure. Both at 0.5 GPa and 1.5 GPa, the reaction rates followed first-order kinetics. In addition, shorter n -alkanes were detected in the reaction products. The results indicate thermal cracking reaction of n -C₂₅ alkane with a free radical chain mechanism, also observed at a lower pressure of 12 MPa (Behar and Vandenbroucke 1996). In addition, various heavier hydrocarbons were detected, which were expected to be formed by polymerization. Details of the reaction mechanism as well as the effects of pressure on the reaction will be discussed in the presentation.

Keywords: Deep carbon cycle , hydrocarbons, GC/MS