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The Hydrogen Resource Potential and Sweet Spots in Hydrocarbon Source Rocks

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Hydrogen (H_2), as the most energy-dense gas and a lower-carbon fuel, plays a vital role in the global energy transition. Traditionally, H_2 is produced from the gasification of coal, steam reforming of natural gas, and electrolysis of water. Over the past few years, however, there has been substantial growth in the exploration of naturally occurring H_2 across all continents, focusing mainly on inorganic origins such as serpentinization processes or the radiolysis of water.

Numerous open- and closed-system pyrolysis experiments, mimicking hydrocarbon generation from organic-rich shales and coals, demonstrated that considerable amounts of H_2 can be generated from the kerogen in source rocks at elevated temperatures. Published data as well as our pyrolysis experiments indicate that open pyrolysis systems are more efficient in generating greater quantities of H_2 compared to closed-system pyrolysis, sometimes even yielding more H_2 than methane. The H_2 liberated from aromatization and condensation reactions of kerogen structures during maturation cannot escape from the closed system and will be consumed in ring-opening and free radical reactions during subsequent secondary cracking. Furthermore, the presence of sulfur in subsurface formations – whether in the form of organosulfur compounds within kerogen or as pyrite in shale – represents an additional H_2 sink due to the formation of H_2S, which has been observed in both geological and laboratory settings.

We propose a novel methodology for assessing the resource potential of H_2 from hydrocarbon source rocks, comparing open-*versus* closed-system pyrolysis experiments. Kinetic parameters governing the generation of hydrocarbons as well as H_2 and other non-hydrocarbon components can be derived from the pyrolysis data. Kinetic modeling integrated into basin modeling enables the determination of the optimal maturity window for H_2 generation. With reconstructed thermal and burial histories, this maturity window can be converted to a subsurface zone with specific depth ranges or temperature intervals conducive to H_2 accumulation, favoring areas of high maturity and low sulfur content of the source rock formations. A practical workflow has been established, building upon pyrolysis and modeling outcomes, to identify prospective "kitchens" and "sweet spots" for the organically sourced H_2 in sedimentary basins.