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QUANTITATIVE ASSESSMENT OF GAS GENERATION, ORIGIN, AGE, AND PALEO FORMATION TEMPERATURE IN PETROLEUM SYSTEM

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The physical properties and generation processes that control natural gas accumulation are distinctly different from those related to oil generation, and require the development of new tools and strategies in order to create effective gas exploration programs. In contrast to the large amount of geochemical information that is preserved in crude oil, natural gas is compositionally very simple and requires creative approaches for maximizing the value of the available data. In the past few years, we have developed two techniques that allow fundamental questions of gas generation, origin, age of formation, temperature of gas generation, and accumulation to be quantitatively addressed. First model is based on first principle (Quantum Chemistry) to predict the most critical properties for gas generation and accumulation such as isotope fractionation patterns, temperature and maturity of the gas source rock, gas quality (e.g., wetness), and the gas to oil ratio (GOR). The experimental foundation of this model is the laboratory pyrolysis, e.g. by integrating with basin modeling tool, one can extrapolate gas isotopic fractionation under laboratory condition to geological frameworks. Second method is to develop a novel optical isotope measurement so we can detect the $^{13}CDH_3$ concentration in the natural gas system. We have synthesized the $^{13}CDH_3$ compound which has obtained all detail line spectrum. The concentration of $^{13}CDH_3$ relative to the normal carbon ($\delta^{13}C$) and (δD) may provide critical information about gas generation condition, environment, age and temperature of gas generation. Based on the Gibb's free energy calculation from first principle (quantum mechanics density function theory), we have quantified the thermodynamic equilibrium of isotopmers. At the current stage, it is not clear whether the natural gas will be randomly populated or it might exactly follow the equilibrium conditions. However, the relative concentration change in $^{13}CDH_3$ will provide us with valuable information about gas formation temperature (paleothermometer). For example, if we choose a gas with a carbon isotopic composition of -47‰ and a deuterium isotopic composition of -120‰, then this gas could potentially be generated by one of three different sources. One possibility might be from a mixture of biogenic and shale gases. Secondly, it is possible to generate such isotopic compositions from early shale gases. Lastly, this could also be generated from secondary cracking of oil. This uncertainty could be further resolved if we can measure the concentration of $^{13}CDH_3$. By determining the gas formation temperature and integrating with other geologic data, it is possible to determine other information about the origin of the gas (Figure 1).

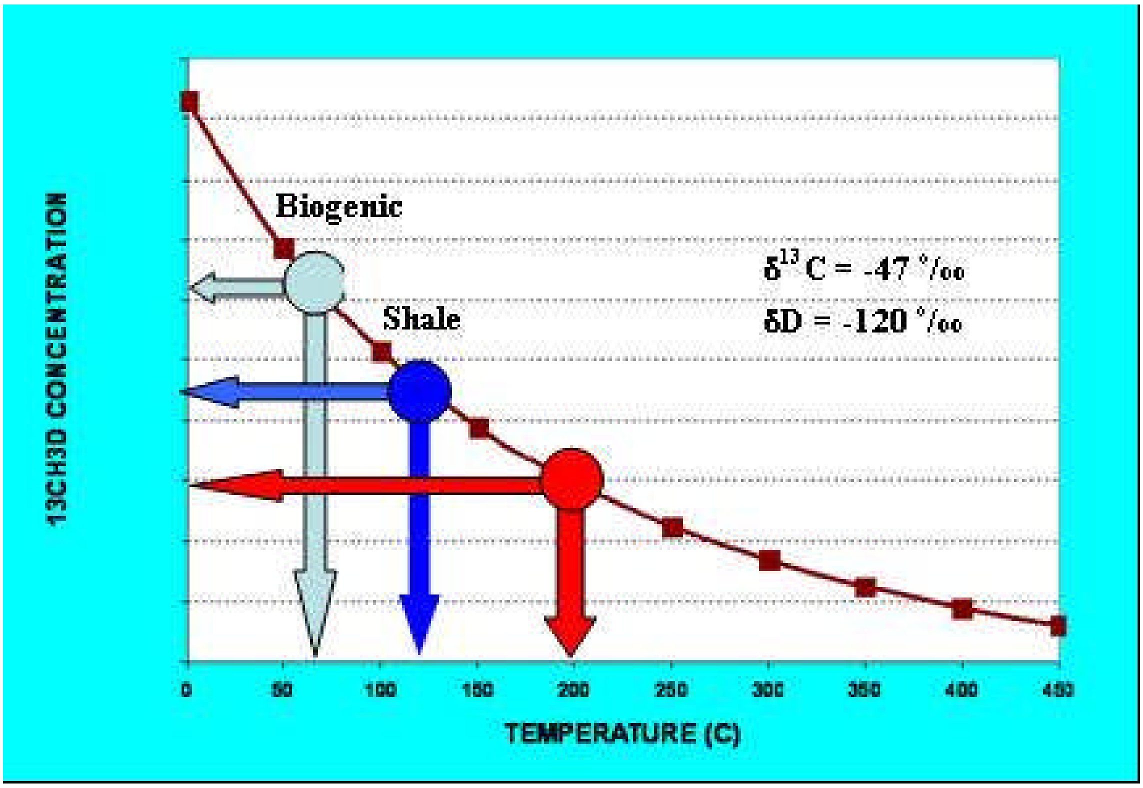

Figure 1. Applications of doubly-substituted methane isotopomer to distinguish the origin of natural gas