



Contribution ID: 700

Type: Oral 20 Minutes

## Sorption of Methane and Carbon Dioxide in Type II-A Kerogen Rough Slit Nanopores by Molecular Simulations

*Monday, 14 May 2018 11:54 (15 minutes)*

Shale gas has redefined energy landscape[1]. The United States (U.S.) natural gas production is expected to increase every year, and in 2035 the U.S. shale gas production may raise to 50% of the total gas production.

Shale rock consists of micropores and mesopores[2]. It is also composed of inorganic minerals (quartz, clays, calcites, and feldspars, etc.) and organic matter (kerogens and bitumens). The organic matter is mainly composed of kerogens and it is considered as the main gas trapping of methane[3] and shows high capacity for carbon dioxide adsorption trapping[4]. An understanding of shale kerogen adsorption characteristics, under the reservoir condition, is required to successfully exploit the shale formations.

Three different types of kerogen depending on its origin can be distinguished: i) type I from a lacustrine anoxic environment, ii) type II from marine shale and continental planktons, and iii) type III from plants in tertiary and quaternary coals. All these types can be classified according to the elemental ratio of Hydrogen/Carbon (H/C), Oxygen/Carbon (O/C), and Sulfur/Carbon (S/C). The physicochemical properties (structure, adsorption, retention, etc.) of the kerogen strongly depend on its origin and on the burial history of the reservoir where it came from[5].

Molecular simulations allow a detailed picture of the structure, thermodynamics and dynamics of the fluid at the interface. In this work the dry structures of type II immature kerogen with different types of dummy particles are simulated. Then, the kerogen media are used to study the sorption of methane and carbon dioxide in the kerogen matrix and at the kerogen rough slit nanopore surface. Our results are compared with the available experimental data.

### References

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**Session Classification:** Parallel 1-E

**Track Classification:** MS 1.32: Sorption, Phase Behavior, and Fluid Transport in Fractured Black Shales