



U.S. DEPARTMENT OF
ENERGY
Office of Science



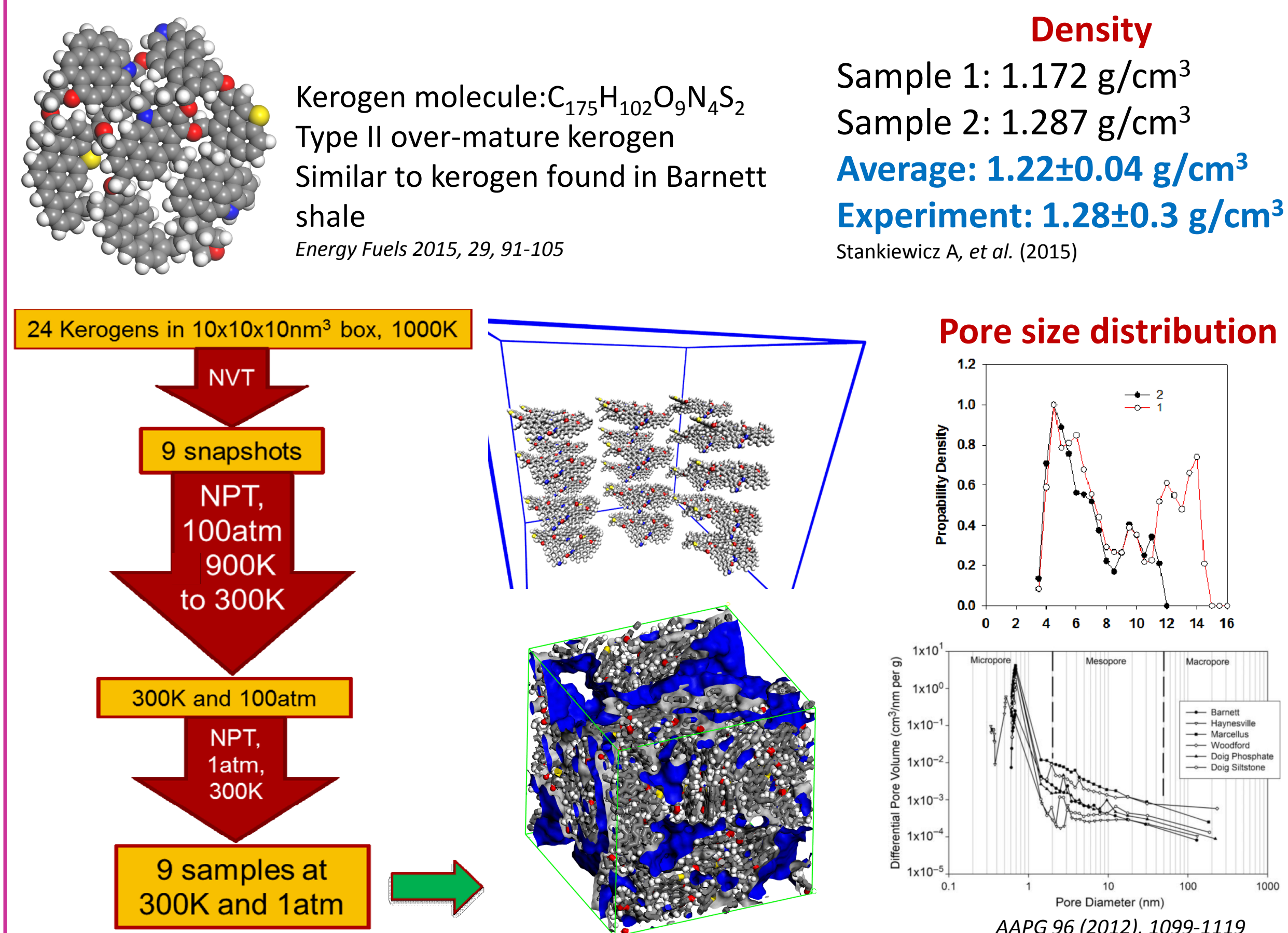
Differential retention and release of CO₂ and CH₄ in kerogen nanopores from molecular simulations

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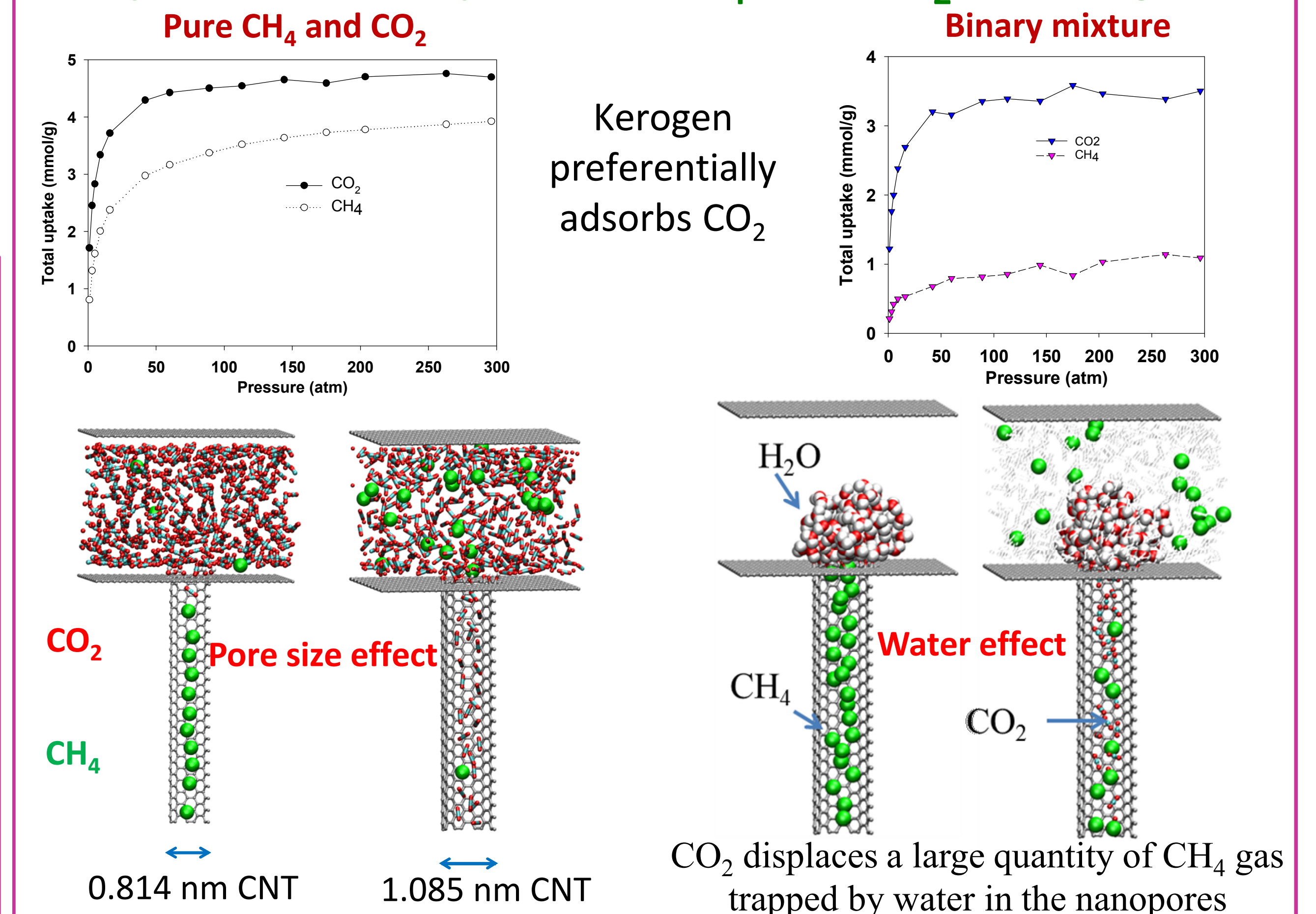
Objective

Understanding nano-structural properties of subsurface porous media including kerogen and clay, and gas adsorption and transport in subsurface porous media.

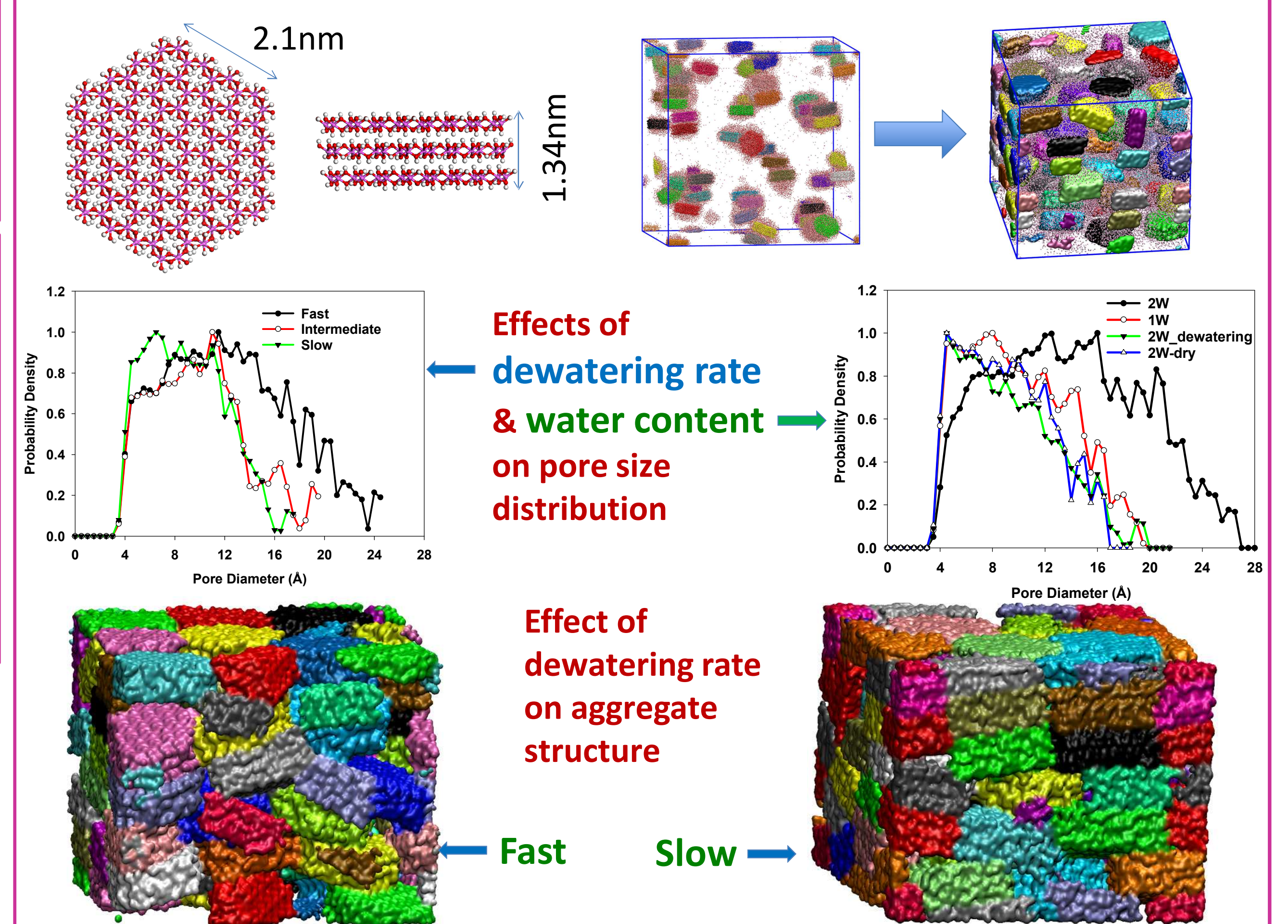
Formation of condensed kerogen



Competitive adsorption of CH₄ and CO₂ in kerogen



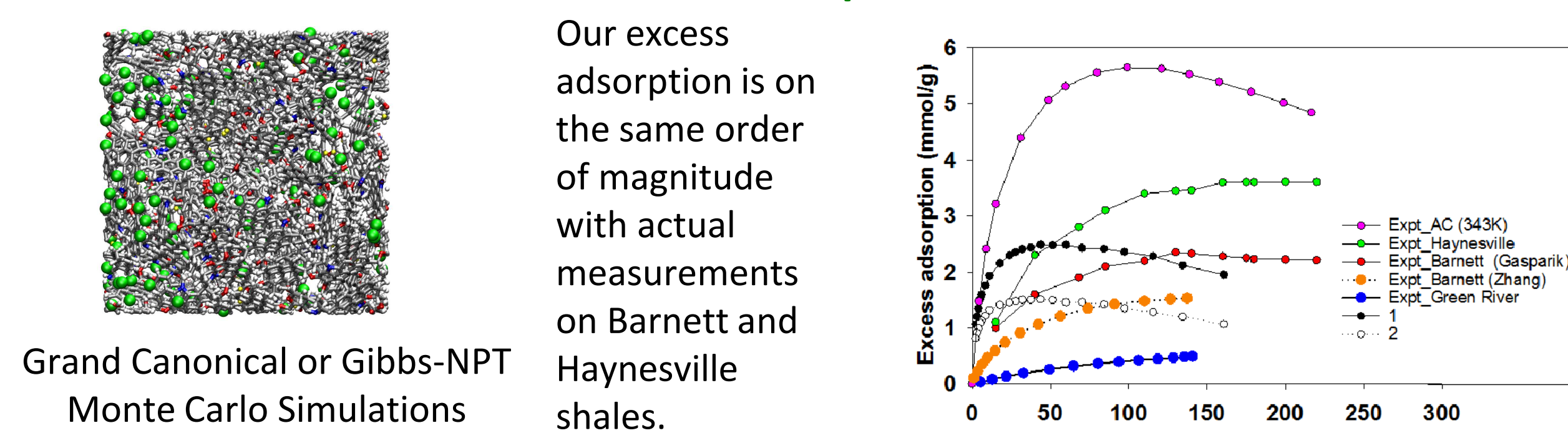
Nano-structural properties of clay aggregates



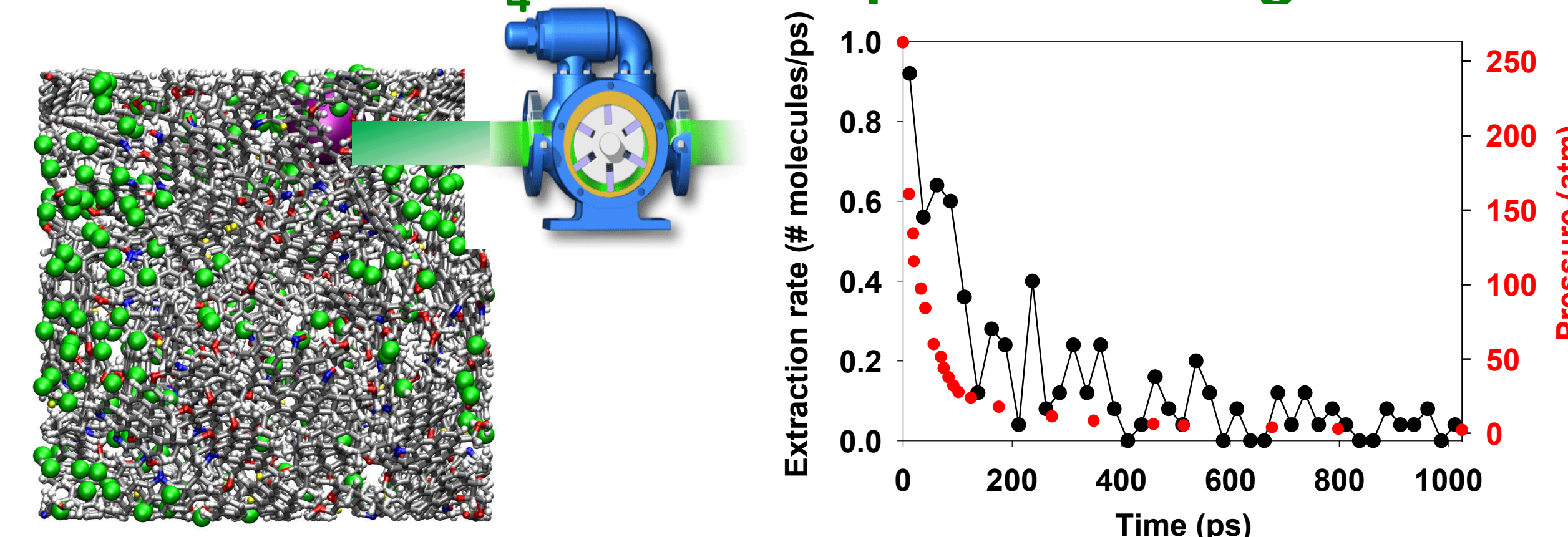
Conclusions

- Methane release from kerogen matrix is characterized by fast release of pressurized free gas followed by slow release of adsorbed gas. A significant amount of gas deposited in kerogen can be trapped in isolated pores and thus not recoverable. (*Sci. Rep. 6, 28053*)
- Kerogen preferentially retains CO₂ over CH₄. When water is present in the kerogen matrix, it may block CH₄ release. However, the addition of CO₂ to a matrix may enhance CH₄ release because CO₂ can migrate through water and exchange for adsorbed methane.
- Dewatering and water content affect micro-porosity of clay aggregates. Slow dewatering will create more compact aggregates compared to fast dewatering. The amount of water present in the clay aggregates strongly affects the particle-particle interactions and hence the clay aggregate structure. (*Sci. Rep. 7, 15286*)

Adsorption isotherm of CH₄ in kerogen



Extraction of CH₄ from nanopores in kerogen



Methane release from kerogen matrix is characterized by a fast release of pressurized free gas followed by a slow release of adsorbed gas.

