

# Numerical study of the impact of organic source rocks' flexibility effects on transport at the nanoscale

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Shale-gas recovery from unconventional reservoirs is a very slow process that exhibits anomalous behaviour at large scales such as non-Fickian productivity declines. Recent studies, focusing on the subnanoporosity of the organic matter called kerogen (where the hydrocarbons are produced and trapped during maturation), has been carried out to elucidate these features [1,2]. Unfortunately, the molecular force field used in these studies is not adapted to capture flexibility effects such as swelling upon fluid adsorption. Those findings are thus restricted to the case of very mature matrices where flexibility effects are negligible. In this work [3,4] we present a re-parameterization of the non-bonded part of the AIREBO C/H potential, achieved to reproduce experimental equations of state for alkane chains, and use it to study the mechanical properties of two - raw and fluid-filled - porous amorphous carbon matrices obtained from quench molecular dynamics simulations, serving as proxies for mature and immature kerogens. While, as expected, the mature matrix is somehow insensitive to pressure and temperature effects, we observe a huge dependence of the density (and thus porosity) of the immature matrix on applied pressure, temperature and fluid loading. Especially, while some open porosity might be observed at atmospheric pressure, the raw immature matrix significantly shrinks in volume at geological pressures (25-100 MPa) where only traces of closed porosity remains. However, the presence of trapped/adsorbed hydrocarbons can significantly open the porosity. As a consequence, the adsorption isotherms for the immature matrix does not plateau at large fluid pressure and simply increases linearly, and the diffusion coefficient increases with the quantity of adsorbed fluid instead of decreasing as in the rigid case.

## References

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