www.cnrs.fr

PRESS RELEASE I PARIS I 01 FEBRUARY 2016

BE CAREFUL ! Embargoed till February 1st, 5pm Central European Time

Molecular models help to better understand shale gas

Although shale gas development is attracting a lot of attention, the recovery method used, hydraulic fracturing, or fracking, is raising increasing concerns. In order to develop more environmentally friendly methods, researchers need models and simulations validated by experiment and capable of reconstructing the complexity of such geological structures. With this in mind, molecular models of kerogen, whose breakdown produces shale gas, have been developed by researchers from the CNRS/MIT International Joint Unit 'Multi-Scale Materials Science for Energy and Environment' and the Institut de Sciences des Matériaux de Mulhouse (CNRS/Université de Haute-Alsace). Such models, derived from experimentally determined properties of kerogen, can be used to investigate the behavior of this organic material. This work is published on the website of *Nature Materials* on 1 February 2016.

Petroleum and natural gas are formed by the breakdown of kerogen, which in turn is produced by the decomposition of organic matter. Although this process can give rise to conventional deposits, it can also take place within highly heterogeneous units such as shales. In this case, the kerogen is compressed within rocks a million times less permeable than in conventional hydrocarbon reservoirs. Temperature, pressure and maturation conditions are still largely unknown, which for now restricts the recovery of the gas they contain to the extraction technique known as hydraulic fracturing, or fracking.

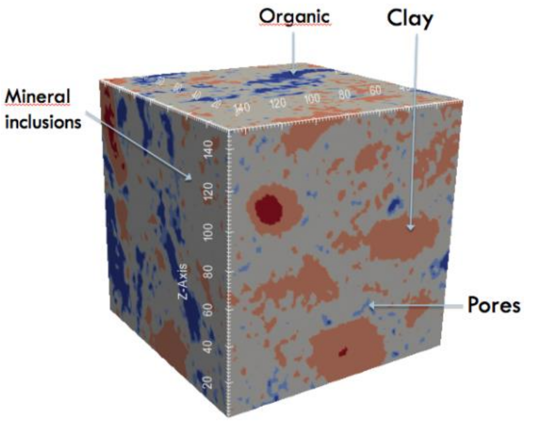
In order to develop new, efficient yet environmentally friendly methods, scientists need new tools. Such tools should enable them to assess the amount and accessibility of resources and improve their understanding of adsorption[1] and transport properties within gas shales. In fact, the researchers applied a hybrid method, combining experiments and simulations, in order to obtain molecular models of kerogens.

To collect data about the chemical composition, texture and density of kerogen, four samples were carefully selected. They differed in their origins and degree of maturation. The researchers studied their characteristics using a wide range of methods, including major facilities such as a synchrotron, in this case the European Synchrotron Radiation Facility in Grenoble, France, and a neutron source (at the Oak Ridge National Laboratory in the US).

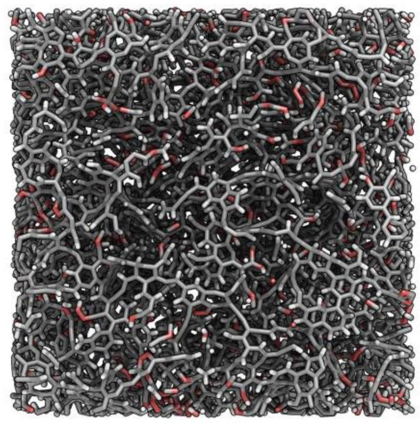
The models obtained were then validated by comparing them with experimentally accessible kerogen properties. They provide a molecular view in a field where samples are generally macroscopic. This work should now help to unravel the microscopic structure of the disordered and heterogeneous materials that

[1] Adsorption is the adhesion of molecules to a solid surface.

make up kerogens, adding one more piece to the arsenal of knowledge that may eventually make it possible to develop shale gas differently.



X-ray microscopy (XRM) image of an untreated sample of gas shale, showing inclusions of pyrite, clay, organic matter and other minerals.
© M. Hubler (MIT) and J. Gelb (Carl Zeiss X-ray Microscopy).



Molecular model of a sample of the Marcellus kerogen studied (the organic phase constitutes the source of hydrocarbons in shale gas). Carbon, hydrogen and oxygen atoms are shown in grey, white and red respectively. The size of the image is 5 × 5 nm. Four samples with different maturities, that is, with different times and conditions of formation, were considered.
© Colin Bousige

Reference

Realistic molecular model of kerogene's nanostructure. Colin Bousige, Camelia Ghimbeu, Cathie Vix-Guterl, Andrew E. Pomerantz, Assiya Suleimenova, Gavin Vaughan, Gaston Garbarino, Mikhail Feygenson, Christoph Wildgruber, Franz-Josef Ulm, Roland J.-M. Pellenq, Benoît Coasne. *Nature materials.* 1 February 2016.
DOI: 10.1038/nmat4541

Contact information

CNRS researcher I Benoît Coasne I **T +33 (0)4 76 51 47 47** I benoit.coasne@ujf-grenoble.fr
CNRS Press Office I Priscilla Dacher I **T +33 (0)1 44 96 46 06** I priscilla.dacher@cnrs-dir.fr