Johns Hopkins University

Department of Chemical and Biomolecular Engineering
Special Seminar

Compressibility of Nanoconfined Fluids: Relating Atomistic Modeling to Ultrasonic Experiments

Presented by Dr. Gennady Gor

ABSTRACT

Fluids confined in nanopores are ubiquitous in nature and technology. In recent years, the interest in confined fluids has grown, driven by research on unconventional hydrocarbon resources -- shale gas and shale oil, much of which are confined in nanopores. When fluids are confined in nanopores, many of their properties differ from those of the same fluid in the bulk. These properties include density, freezing point, transport coefficients, thermal expansion coefficient, and, as it was shown recently [1], elastic properties.

The elastic modulus of a fluid confined in the pores contribute to the overall elasticity of the fluid-saturated porous medium and determine the speed at which elastic waves traverse through the medium. In this talk I will show how elastic modulus of a confined fluid in a nanopore can be calculated based on Monte Carlo and molecular dynamics simulations and illustrate it with calculations for various fluids [2]. Additionally, I will present our recent experimental measurements of elastic properties of water confined in nanoporous glass samples. Our results suggest that some of the models widely used for describing elasticity of fluid-saturated porous solids need to be revised [3].

[1] Dobrzanski, C. D.; Gurevich, B.; Gor, G. Y. "Elastic Properties of Confined Fluids from Molecular Modeling to Ultrasonic Experiments on Porous Solids" Appl. Phys. Rev. 2021, 8, 021317, DOI: 10.1063/5.0024114

[2] Maximov, M. A.; Gor, G. Y. "Molecular Simulations Shed Light on Potential Uses of Ultrasound in Nitrogen Adsorption Experiments" Langmuir 2018, 34(51), 15650-15657, DOI: 10.1021/acs.langmuir.8b02909

[3] Gor, G. Y.; Gurevich, B. "Gassmann Theory Applies to Nanoporous Media" Geophys. Res. Lett., 2018, 45(1), 146-155, DOI: 10.1002/2017GL075321,

BIO

Dr. Gennady Gor received a PhD in theoretical physics from St. Petersburg State University, Russia in 2009. He continued his postdoctoral research in the United States, at Rutgers University, Princeton University and Naval Research Laboratory. In 2016 he joined the Chemical and Materials Engineering department at NJIT as an assistant professor, and was promoted to associate professor in 2022.

Gennady's Computational Laboratory for Porous Materials employs a set of modeling techniques, such as Monte Carlo and molecular dynamics simulations, density functional theory and finite element methods, to study materials ranging from nanoporous adsorbents to macroporous polymers and geological porous media. He authored more than 60 peer-reviewed publications and is the recipient of the National Research Council Associateship (2014) and the NSF CAREER Award (2020).

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