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Molecular dynamics of a fluid confined in kerogen from memory kernels

Thursday, 2 June 2022 15:15 (1h 10m)

The depletion of conventional oil/gas reserves has led to the extensive exploitation of hydrocarbon-rich organic source rocks. However, recovery of hydrocarbons from kerogen, the main organic component of shales, has proved to be complicated due to the strong impact of kerogen microporosity on fluid transport. In order to understand the nature of solid-fluid couplings and its impact on fluid production/storage, a multiscale approach including advanced numerical and statistical methods should be applied. As a step towards this goal, we investigated the fluid dynamics which was affected by the solid dynamics through the application of molecular dynamics (MD) simulations and coarse-graining procedures based on the generalized Langevin equation. In this framework, the influence of the solid (kerogen) on the fluid flow is incorporated in the so-called noise, of which the autocorrelation function (ACF) is the memory kernel. To compute memory kernel, the post-treatment of trajectories from molecular simulations of fluids confined in rigid and flexible kerogen have been performed using two coarse-graining techniques, one based on the inversion of the Volterra equation of the second kind [1] and the other one based on the reconstruction of the backward orthogonal dynamics [2]. The latter method also gives access to the noise on top of the memory kernel while being computationally expensive. These approaches have allowed us to extract the feedback of the solid dynamics on the fluid one. It has been proven recently by a study on the memory kernel that, in the case of a bulk fluid, hydrodynamic modes govern the fluid dynamics even for colloids of molecular size [2]. In contrast, hydrodynamics is inadequate to describe the transport of a fluid trapped in rigid pores of a kerogen molecular model [3,4]. Interestingly, the kerogen flexibility does not contribute to the cross-correlations between fluid molecules at long times leading to purely diffusive behavior. Nevertheless, our study has shown that the velocity ACF (VACF) scales exactly the way predicted by the hydrodynamic theory for both rigid and flexible solid cases despite negligible collective effects in fluid diffusion. The similar decay of the VACF has been determined by Lesnicki et al. for a tagged particle in a fluid [2]. All of that lead to the assumption that this scaling of the VACF (~t-3/2) at long times is not restricted to hydrodynamics. Moreover, our analysis of memory kernel has shown that its decay does not follow the long-term trend prescribed by the hydrodynamics. Combining MD simulations with the memory kernels investigation will contribute to a more profound understanding of the impact of the environment (polymers, water, etc.) on confined fluid dynamics.

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References

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Time Block Preference

Time Block B (14:00-17:00 CET)

Participation

In person

Primary authors: Ms ARISKINA, Kristina (Laboratoire des Fluides Complexes et leurs Réservoirs, UMR 5150, E2S UPPA); Prof. GALLIERO, Guillaume (Laboratoire des Fluides Complexes et leurs Réservoirs, UMR 5150, E2S UPPA); Dr OBLIGER, Amael (Institut des Sciences Moléculaires, UMR 5255, Université de Bordeaux/CNRS)

Presenter: Ms ARISKINA, Kristina (Laboratoire des Fluides Complexes et leurs Réservoirs, UMR 5150, E2S UPPA)

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