Contribution ID: **510** Type: **Oral Presentation**

Pore networks meet computational chemistry: a hybrid approach for studying the flow of fluid mixtures under various thermodynamic conditions in nanoporous materials.

Thursday, 2 June 2022 09:40 (15 minutes)

An unconventional reservoir is a multiscale system in which pores with the size of several nanometers can reach 80% of the total pore volume. [1]. Traditional methods of production processes modeling based on the Navier-Stokes equation, which describes the behavior of a continuous medium, are not suitable for this case, since they do not consider the molecular interactions of fluid and rock. In nanopores the interaction of fluid molecules with solid surface significantly affects the component composition, thermodynamic, phase and transport properties [2 - 4]. The development of technologies for effective production and design of enhanced oil recovery methods requires new approaches to modeling and understanding of the processes occurring at the molecular level. A wide range of phenomena occurring at the nanoscale can be investigated using Molecular Dynamic (MD) modeling. However, since MD requires the numerical solution of the equations of motion for a system of interacting particles, the method is computationally expensive, and the calculations could take from several hours to several days [5]. To accelerate the calculation of the equilibrium state of the fluid in a multiscale pore system, a new hybrid approach is proposed. To study the behavior of hydrocarbon and carbon dioxide mixtures in nanoporous media a new method that combines modern Density Functional Theory (DFT) and MD with flow simulations in Pore Network models was developed in the current work.

At the first stage of the proposed method, the distribution of the component composition in micro- and nanopores and the equilibrium thermodynamic parameters is determined using DFT. Then, in the second step, a MD calculation of the system is conducted with the previously determined distribution of component composition between micro and nanopores. MD is used to calculate the fluid flow in the pore space and effective transport properties, considering the distribution of fluid components. Since the equilibrium distribution of the components in nanopores is calculated at the first stage, the time for calculating the transport properties will be significantly less than the time for direct MD simulation. Further, the transport and filtration properties of the entire porous medium are described and modeled based on the pore-network approach, taking into account the thermodynamic effects in nanopores.

As a result, we developed a multiscale technique for modeling and studying the properties of fluid mixtures in porous medium, depending on the thermodynamic conditions and the component composition of the fluid. The proposed method was applied to calculate the properties of various mixtures of hydrocarbons and carbon dioxide in nanoporous materials, so case studies are discussed in detail.

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Time Block Preference

Time Block C (18:00-21:00 CET)

Participation

Unsure

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