Contribution ID: **44** Contribution code: **Board 61** Type: **Poster Presentation**

A unified approach for bridging the gap between cDFT and equation of state for confined fluids

Monday, May 20, 2024 7:10 PM (20 minutes)

In recent years, extensions of the cubic equations of state for fluids confined in different geometries have been developed based on the Generalized van der Waals Theory. These equations make it possible to describe the Helmholtz energy as a function of temperature, volume, and number of components, from which expressions for all other thermodynamic properties can be derived. Extending the Equation of States to represent confined fluids in micro and mesopores is still challenging. Although different authors have modified classical expressions like Peng-Robinson1 to model adsorption, these models usually reduce the pore structure to simple geometries and pore potentials. Depending on the level of simplification, the methodology can struggle when representing systems in a range of temperatures. Although they have a lower computational cost, they still do not have the robustness seen in methods such as Monte Carlo (MC) simulations or those based on the classical density functional theory (NLDFT). However, MC and NLDFT are the most recommended for micro and mesopores, but it is challenging to use them to obtain thermodynamic properties for fluids in larger pores, generating a demand for a single methodology that covers all scales. Therefore, this work simulates pore confinement with an NLDFT model and uses the fluid physicochemical properties to feed the Peng-Robinson extended to represent the confinement effect. To verify the success of this approach, we carried out CO2 adsorption isotherms on faujasite zeolite in a magnetic suspension balance (Rubotherm) over a pressure range of up to 50 bar. The results show that when we feed this NLDFT information into the equation of state for a confined fluid, the resulting model can more adequately represent the CO2 isotherms in faujasite at different temperatures (Figure).

Primary authors: Prof. GOMES BARRETO JR., Amaro (Universidade Federal do Rio de Janeiro); Dr CARRIJO DE MELO, Dárley (CENPES/Petrobras S.A.); Mr ROCHA PINTO, Felipe (Universidade Federal do Rio de Janeiro); Prof. WANDERLEY TAVARES, Frederico (Universidade Federal do Rio de Janeiro); SERMOUD, Vítor (Federal University of Rio de Janeiro)

Presenter: Prof. GOMES BARRETO JR., Amaro (Universidade Federal do Rio de Janeiro)

Session Classification: Poster Session

Track Classification: Poster Presentations