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HIGHLIGHTS IN ENERGY RESEARCH

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Understanding the role of thermophysical properties to design efficient processes for CO2 capture and separation

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One of the alternatives to mitigate CO2 emissions is to capture and separate it from diluted sources before it is emitted into the atmosphere. The first step in this process is to find suitable CO2 capture technologies, being aqueous monoethanolamine (MEA) solutions the most mature technology for this purpose currently used in industrial processes. However, this process has some important drawbacks such as high regeneration energy consumption, loss of solvent and amine degradation. Different strategies are devised to overcome these limitations, all of which require the fundamental understanding of the key molecular properties leading to the desired performance. The focus of this presentation will be on how understanding the molecular interactions of complex mixtures can help in the development of more efficient processes for CO2 capture and separation. We will present the capabilities of a robust molecular-based equation as a screening tool of chemical solvents for the efficient removal of CO2 from industrial gas streams. The tool is built based on the soft-SAFT equation in which substances are modelled as chain molecules characterized by a set of molecular parameters representing the chemical structure of molecules and key intermolecular interactions. The equation provides accurate phase equilibria, interfacial properties and viscosities of the relevant mixtures allowing predictions of their performance at process conditions, with a very limited set of experimental data. The study is performed in a systematic manner, first benchmarking the performance of the model for capturing CO2 in aqueous amines, followed by water-free and water-lean amine systems. In addition, results from molecular simulations performed to understand the effect of degraded amines in the capture and separation process will also be presented. Finally, examples will be provided on combining molecular simulations with process modeling for designing ad-hoc processes of CO2 separation by adsorption as an alternative to aqueous amines.

Bio Prof. Lourdes Vega : Born in 1965 in Villanueva del Fresno, Badajoz, Spain, she obtained her Ph.D. in Physics from the University of Seville, Spain, in collaboration with the Chemical Engineering Department, University of Southern California, USA. She has developed her career between academia and industry, with positions in the USA (Cornell University, University of Southern California), Spain (Universitat Rovira I Virgili, Consejo Superior de Investigaciones Científicas - CSIC) and the UAE. She was the General Director of MATGAS, Technology Director of Air Products & Chemicals and Founder and CEO of AlyaTech. Currently she is a Professor and Director of the RICH Center at Khalifa University in Abu Dhabi, UAE. Prof. Vega is an internationally recognized expert in combining molecular modeling with advanced experimental techniques for clean energy and sustainable products.