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SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

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Why implementation of multiscale simulation strategies to screening porous materials for adsorption applications is (so) challenging

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The discovery of new classes of porous adsorbents such as metal-organic frameworks (MOFs) has opened access to a very large number of porous structures with a wide range of functionalities, which can be potentially exploited in different separation applications. Experimental evaluation of all these materials for specific applications is not feasible, and as a result, this prompted the development of high throughput computational screening methods.

In this presentation, I will reflect on the development of the multiscale strategies that combine molecular simulations and pressure swing adsorption modelling and optimization to predict performance of the materials on the process scale. Specifically, I will focus on the challenges associated with the interface between molecular and process levels of description and demonstrate that the emerging picture is quite complex. As a case study, a well-known 4-step vacuum swing adsorption (VSA) cycle with light product pressurization (LPP), and Zeolite 13X as adsorbent in application to carbon dioxide removal from a typical flue gas stream (15% CO_2, 85% N_2, 1 atm) will be considered. I will discuss (a) the effect of the protocol for fitting experimental adsorption data with analytical adsorption models (e.g. dual-site Langmuir model), (b) influence of the pellet porosity and (c) influence of the pellet size on the process performance and material raking. Another aspect of the multiscale strategies we intend to explore is the accuracy of the molecular force fields, particularly in reproducing nitrogen isotherms, and how this affects predictions for the performance of the material in a process and the resulting ranking.

CV: Prof. Lev Sarkisov

Prof. Lev Sarkisov obtained PhD in Chemical Engineering from the University of Massachusetts (Amherst, USA) in 2001. Following postdoctoral research posts at Northwestern (2001-2003) and Yale Universities (2003-2005), he joined the University of Edinburgh in 2005 as a Lecturer in Chemical Engineering. He was promoted to Senior Lecturer in 2010 and Professor in 2017 with the Personal Chair in Molecular Thermodynamics, and became Director of Discipline in Chemical Engineering (equivalent to the Head of the Department) in 2018. Prof. Sarkisov's group specializes in multi-scale approaches to design of novel, functional porous materials for carbon capture, sensing, energy storage and drug delivery; multi-scale approaches to engineering chemical processes; adsorption and membrane separation processes, molecular simulations in application to chemical engineering problems.