

Systems Analysis of Membrane Reactors for Energy Applications and Process Intensification

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With the growing energy demand and stringent environmental regulations, the efficient, economic and sustainable use of major energy sources has become increasingly important. The development and implementation of novel technologies for the improved utilization of such energy sources can be accelerated by the use of process systems engineering tools, such as process modeling, design, control, and optimization. In particular, the investigation of intensified methane conversion routes with reduced cost and minimized environmental impact is especially motivated by the presence of abundant amounts of natural gas in the different shale formations in the country, including the Marcellus Shale in West Virginia. This presentation will focus on the systems analysis of natural gas utilization routes for the production of fuels and chemicals. The use of membrane reactor (MR) processes for the direct methane aromatization (DMA) conversion to hydrogen and benzene will be the main route of interest. The presentation will also address the systems analysis for the application of MRs to other energy systems such as the oxidative coupling of methane (OCM) for ethylene production and the water gas shift (WGS) reaction for carbon capture in advanced coal-fired power plants.

In the last decades, MRs have emerged as examples of intensified processes as they combine reaction and separation unit operations in one process improving the system efficiency and lowering the cost. Specifically, in the DMA-MR process, higher methane conversion than in conventional reactors is enabled due to the selective hydrogen removal from the reaction side through the membrane. This removal shifts the reaction equilibrium towards the products, thus increasing methane conversion and benzene production rate. The nonlinear and multivariable nature of the DMA-MR system associated with the reaction-transport phenomena interplay make this system challenging to design and optimize. This presentation will introduce a novel operability-based approach for design and intensification of processes described by complex nonlinear models. The developed operability approach is based on nonlinear programming tools and describes the relationship between the key process input (e.g., membrane selectivity and permeance, reactor length and diameter) and output (e.g., methane conversion and benzene production rate) variables through a nonlinear mapping obtained by employing the process model. The results of the operability analysis demonstrate the promising capabilities of the developed approach to provide guidelines for experimental research. These results also show that the application of the operability method as a tool for process intensification enables the reduction of the DMA-MR footprint ($\approx 77\%$ reactor volume and 80% membrane area) for an equivalent level of performance when compared to the base case.