

Hydrocarbons are Separated and Purified using Porous Materials

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Abstract

In addition to the chemical and petrochemical industries, hydrocarbons are crucial to the global energy system. They are crucial feedstock for the creation of many of our chemical products and materials, including pharmaceuticals, coatings, and plastics. They are not only significant fuels, such as gasoline, diesel, and kerosene but also critical materials. However, hydrocarbons derived from crude oil or natural gas are almost usually mixed that must be separated and refined into a single component to be used in the creation of other products, such as plastics. It is still difficult to separate hydrocarbons with similar sizes and molecular structures, and consequently similar physicochemical properties. Technologies for separation based on adsorbents have the potential to replace the current industrial practice of cryogenic distillation.

Keywords: Hydrocarbon separation, metal-organic frameworks, porous organic frameworks, Porous materials zeolites

Introduction

The role of natural gas in the global energy system is expanding. According to reports, in 2018 the world's natural gas consumption increased by 5.3%, which is one of the highest rates of growth since 1984 [1]. The demand for natural gas on a global scale has also increased significantly along with rising standards of life and associated consumption. Methane is the main component of natural gas, although it also contains a variety of impurities, such as N₂, CO₂, water, hydrogen sulfide, and other sulfur compounds.

To achieve pipeline criteria, typically >90% methane, all raw natural gases containing these pollutants must undergo some sort of treatment. In addition, the availability of natural gas has increased significantly as a result of the development of unconventional sources such as shale gas, coalbed methane, landfill gas, and methane from anaerobic wastewater treatment facilities [2]. These sources are now crucial in bridging the supply-demand gap for natural gas. Water, nitrogen, carbon dioxide, and sulfur are typically encountered contaminants in such unusual natural gases. These impurities must be eliminated to increase the natural gases' purity and energy content. One of the most difficult and crucial separations for the use of natural gas is the CH₄/N₂ separation because of the close physicochemical similarities between CH₄ and N₂ [3].

The separation of xylene isomers and olefins from paraffin. The most frequently produced synthetic plastics in the world, polyethylene, and polypropylene, are made from the essential petrochemical feedstocks ethylene and propene. The process of steam cracking hydrocarbons ranging from ethane to vacuum gas oils, in which ethene and propene coexist with numerous other hydrocarbons including ethane and propane, typically yields ethene and propene. Ethane and propane must be removed since the creation of PE and PP requires polymer-grade (>99.5%) ethene and propene [4].

Currently, the energy-intensive cryogenic distillation method is used to separate ethene from ethane and propene from propane. This process is carried out in massive columns with more than 100 trays. Adsorption-based separation is thought to be a more effective and affordable alternative technique to carry out this very energy-intensive operation. The three xylene isomers para-ortho, meta-xylene, as well as ethylbenzene, make the C₈ aromatics, which serve as the starting point for the synthesis of numerous

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significant chemical intermediates. The raw material used to create terephthalic acid is the most valuable aromatic because terephthalic acid serves as the primary precursor for the creation of polyester and Polyethylene Terephthalate (PET) [5].

Since there are so many porous materials finding optimal and promising adsorbents quickly might be challenging. The rapid evaluation and rational design of adsorbents have become possible thanks to High-Throughput Computational Screening (HTCS) [6]. One screening method is high-throughput screening with molecular simulation or DFT calculations, which has been crucial in quickly identifying promising structures and accurately assessing the adsorption and separation performances of porous adsorbents.

This screening strategy would waste enormous computational resources, as well as valuable research time, due to the accumulation of enormous volumes of simulated data and the quick growth of adsorbents (primarily MOFs). A different high-throughput screening strategy based on machine learning that can resolve the aforementioned issues by training data has gradually gained more attention [7].

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