Optimizing Natural Gas Separation and the Haber-Bosch Process with Thermally Rearranged Polymers: Effects of Morphology and Chemical Structure on Free Volume and Transport Properties of HAB-6FDA Structures

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Natural gas separation and ammonia purge gas recovery are among the most important industrial processes by accounting for 22% of all in-plant energy use and improving the Haber Bosch process, respectively. Current gas separation technology is largely energy intensive, corrosive, and costly. Thermally rearranged (TR) polymers are a new class of polymer membranes that are highly effective for applications in gas separations, yet the cause of their effectiveness is largely unknown. In this study, polyimides and polybenzoxazoles derived from HAB and 6FDA were used to determine factors that contribute to the separation properties of TR polymers. For the first time, effects of morphology (packing of polymer chains) and chemical structure of molecules on free volume was investigated with isothermal studies of the TR process by tracking the permeability and selectivity for a variety of partially converted samples. Polymers were tested according to treatment temperature and holding time. Along isotherms, increases in effectiveness varied. Free volume increased along isotherms. FTIR identified samples with identical chemical structures but differing transport properties, attributable to free volume, which varied by as much as 20%. The conclusion of this work was that morphology plays a vital role in the effectiveness of TR polymers. These findings help identify parameters that be tweaked to improve natural gas separation, nitrogen enrichment, and ammonia purge gas recovery (which can improve the Haber process, the producer of over 500 million tons of nitrogen fertilizer yearly. This finding will lead to cost savings, cleaner energy and safer gas separation processes.

Awards Won:

Second Award of $2,000