Integrated MOF and P/VSA Process Design: Descriptor Optimization

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Abstract

An integrated metal-organic framework (MOF) and pressure/vacuum swing adsorption (P/VSA) process design framework is presented for gas separation. It consists of two steps: descriptor optimization and MOF matching. In the first step, MOFs are represented as a large set of chemical and geometric descriptors from which the most influential ones are selected and treated as design variables. The valid design space is confined using a tailored classifier model and logic constraints. Based on collected adsorption isotherms of 471 different MOFs, data-driven isotherm models are developed. Combining the design space, isotherms, and process models, an integrated MOF and P/VSA process design problem is formulated. MOF descriptors and process operating conditions are optimized to maximize the process performance. The obtained optimal descriptors and isotherms can be used to guide the discovery of high-performance MOFs in a subsequent MOF matching step. This article addresses the first descriptor optimization step exemplified by propene/propane separation.

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