

Integrated metal-organic framework (MOF) and pressure/vacuum swing adsorption process design: MOF matching

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Abstract

A two-step integrated MOF and pressure/vacuum swing adsorption (P/VSA) process design has been recently established for gas separation. In the first step, selected MOF descriptors and process operating conditions are simultaneously optimized to maximize the process performance. Based on the obtained results, the second step (i.e., MOF matching) is addressed and exemplified by propene/propane separation in this work. Computational MOF synthesis and screening are carried out to find new advanced material candidates for enhancing the separation process efficiency. First, model-based property-performance relationships are developed for fast MOF screening. Then, MOF building blocks are extracted from 471 CoRE MOFs. With these building blocks, 45472 hypothetical MOFs are created. After model-based and molecular simulation-based screening, six candidates are left and sent to P/VSA process optimization. Finally, three candidates are found to meet the pre-defined separation specifications and one candidate shows a better process performance than the best out of the 471 MOFs.

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