Extended Abstract
Volume 9:4, 2021

Biodiversity & Endangered species

Open Access

Impacts of entropic separation effects

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Abstract

Mitigating the impact of climate change and striving for appropriate resource and raw material management are two of the most pressing issues of our time. Industrial processes must also be adjusted in order to achieve those goals. This development must, among other things, try to replace non-sustainable practises with environmentally beneficial ones. Adsorption technologies could be used to replace unsustainable techniques like distillation in order to separate hydrocarbons. Metal-organic frameworks are good candidates for conducting extremely efficient adsorption procedures to separate hydrocarbons because of their high surface-to-volume ratio and the vast range of options for designing and modifying the pore environment. However, for a wide range of industrial applications, a thorough understanding of separation effects and the behaviour of guest molecules within metal-organic framework channels is required. Apart from the well-known separation processes based on enthalpic, kinetic, or steric (i.e., sieving) differences, there is a third process based on entropic effects that appears to be virtually unknown and, as a result, is frequently overlooked. The efficiency with which guest molecules can organise themselves inside the channels of nanoporous materials is described by these entropic effects. Entropic separations are of particular importance because of the high selectivities that can be achieved. The goal of this talk is to provide a brief overview of entropic separation effects and to demonstrate individual results from Monte Carlo simulations of entropic hydrocarbon separation.

Adsorption techniques based on metal-organic frameworks --â€“ or nanoporous materials in general- There is another separation process based on entropic differences, in addition to the well-known separation methods based on enthalpic, kinetic, or steric (i.e., sieving) differences. The efficiency with which guest molecules can be organised within the channels of nanoporous materials is described by these entropic effects. They can lead to surprising selectivities in some circumstances [1-3]. Regrettably, these impacts are rarely considered and appear to be essentially unknown.

The goal of this research is to contribute to a better understanding of entropic separation effects and to identify potentially intriguing metal-organic frameworks capable of solving separation problems efficiently using entropic effects. To that purpose, grand-canonical Monte Carlo simulations were used to calculate the adsorption isotherms of a variety of hydrocarbon mixtures for a variety of metal-organic frameworks, as well as visualise the organisation of the examined guest molecules within the channels of those materials. Grand-canonical Monte Carlo simulations were used to determine the adsorption isotherms of a range of hydrocarbon mixtures for a number of metal-organic frameworks, as well as visualise the organisation of the investigated guest molecules within those materials' channels.

This work is partly presented at 3rd International Conference on Materials Science and Engineering October 07-08, 2019 | Frankfurt, Germany