Prediction of the breakthrough performance of "gating" adsorbents using osmotic framework adsorbed solution theory

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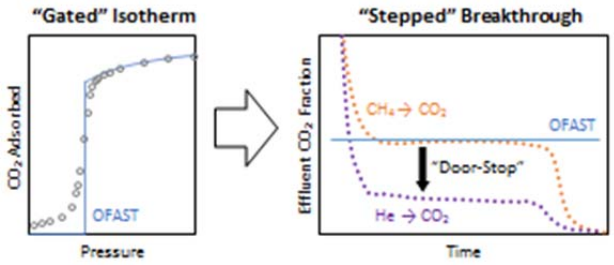
An experimental and theoretical study was conducted of the breakthrough performance of the flexible metal-organic framework $Cu(bpy)_2(BF_4)_2$ (bpy = 4,4'-bipyridine), termed ELM-11. Pure CO_2, He, and N_2 gases, as well as binary gas mixtures of these species, were used to perform breakthrough column experiments on ELM-11, a soft porous crystal that possesses both a highly ordered network and structural transformability[1]. ELM-11 exhibits a stepped breakthrough curve for CO_2 not seen for rigid adsorbents. By comparing the step heights observed in the experimental breakthrough curves with gating pressure predictions obtained from osmotic framework adsorbed solution theory (OFAST)[2], it is shown that the OFAST method can accurately predict the occurrence and height of the steps observed in the breakthrough curves of flexible metal organic frameworks. For specific gas mixtures, the ELM-11 breakthrough curves reveal a "door-stop" type effect[3], wherein the observed step heights for CO_2 breakthrough curves are reduced when the gas mixture contains species that possess a small kinetic diameter, such as helium.



References

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