Chemical Engineering Thesis Defense

Analysis of Non-isothermal Adsorption of Carbon Dioxide in Metal Organic Frameworks

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Abstract

Adsorption is fundamentally known to be a non-isothermal process; in whichtemperature increase is largely significant —causing fairly appreciable impacts on theprocess kinetics. For porous adsorbent particles like MOFs, silica gel, and zeolite,the resultant relative heat generated is partly distributed within the particle; and therest is transferred to the surrounding ambient fluid (air).For large step changes in adsorbed phase concentration, and fast adsorption rates,especially, the isothermality of adsorption (as in some studies), is an inadequate assumption, and inspires rather erroneous diffusivities of porous adsorbents. Isothermalmodels, in consequence, are insufficient for studying adsorption in porous adsorbents.Non-isothermal models can satisfactorily and exhaustively describe adsorption inporous adsorbents. However, in many of the analyses done using the models, thermalconductivity of the adsorbent is assumed to be infinite, thus, particle temperature istaken to be fairly uniform during the process —a trend not observed for CO2 adsorption on MOFs.A new and detailed analysis of CO2 adsorption in a single microporous MOF-5 particle, assuming a finite effective thermal conductivity; along with a comprehensiveparametric study of the process, are presented herein. The corresponding temperature and diffusivity changes are also reported.

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