On the resolution of constant isosteric heat of propylene adsorption on graphite in the sub-monolayer coverage region

ABSTRACT

An early experimental study by Bezus, Dreving and Kiselev [1] on the adsorption of propylene on Spheron-6 carbon black (graphitized at ~3000C) reported a plot of constant isosteric heat versus loading in the sub-monolayer region. This contrasts with their report of a linear increase in isosteric heat for propane, a similar molecule to propylene. In this paper, we report extensive Grand Canonical Monte Carlo (*GCMC*) simulations and a high-resolution experimental study of propylene adsorption on Carbopack F, a highly graphitized thermal carbon black, over the same temperature range studied by Bezus et al. From this combined simulation and experimental study we conclude that propylene also shows a linear increase in the isosteric heat versus loading in the sub-monolayer region, indicating that the linear increase in the fluid-fluid interaction in this region more than compensates for the decrease in the solid-fluid interaction that results from the change in orientation of the adsorbate molecules. Our study contradicts the propylene results of Bezus et al., and careful inspection of their isotherm in the sub-monolayer region shows that it does not follow Henry's law. This calls into question their argument that π-π interactions between propylene molecules are an explanation for the constant heat.

Keyword: Isosteric heat; Propylene adsorption; Graphite; Sub-monolayer coverage region