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New mathematical models for adsorption on heterogeneous surface of carbonaceous adsorbents

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The optimal selection of the methods and conditions for the production of adsorbents requires reliable and accurate description of the parameters of the heterogeneous surfaces and physico-chemical processes occurring on them. Many theories of the adsorption processes were developed in the past century, which assume different mechanisms of processes on surfaces and various simplifications. This work presents the results of the application of new mathematical models with the unique numerical fast multivariate numerical identification procedure as the universal tool for analysing the heterogeneous surfaces. The mathematical models are based on general thermodynamics expressing changes of internal energy ΔH and configurational entropy ΔS due to the process. To derive the formulas for ΔH and ΔS were exploited a BET-like approach, in which the adsorption system is constructed by considering a virtual multistep adsorption. In the proposed model's adsorption process is viewed as a clusterisation of adsorbate molecules in pores, with a cluster size limited by micropore size. A set of pore geometry – adsorption energy relationships is derived and checked by fast multivariant fitting procedure of the model to adsorption data. The proposed models yield a broader range of reliable information on the surface structure of the analysed material, which is particularly useful for the assessment of the impact of production process conditions and modifications on the development of both geometrical and energetic properties of the surface of heterogeneous catalysts.

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