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MODELING OF CO-H_2 GAS STREAM MOTION AT CARBIRIZATION OF CATALYST

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The questions of influence of composition and input speed for stream CO-composing gases in reactionary space on kinetics of their disintegration on ferrous catalytic agents have been considered. It is set pictorial diagram for distribution of carbon concentration in the structure of catalytic agent and carbon monoxide in a gas phase.

Keywords: catalytic agent, carbon single-oxide, hydrogen, gas stream, convection, diffusion

A reaction of dissociation for carbon monoxide $2\tilde{N}\hat{I} \Rightarrow \tilde{N} + \tilde{N}\hat{I}_2$ always is the subject of intent research in connection with the opened perspective of its use for a receipt comparatively cheap carbon with unusual properties.

A research task is research of influence of motion of gas stream $\tilde{N}\hat{I} - \acute{I}_2$ on kinetics of carburization of metals of group of iron and distribution of concentration of carbon and carbon monoxide by modeling method.

For the study of influence of composition and speed of supply of gas stream in reactionary space at carburization of catalyst there are applied the mathematical package «Femlab 2.3». In calculations there are allow the modes of diffusion in a solid body and also modes diffusion and convection in a gas phase.

There is worked out the microscopic model of co-operation of gas stream with the surface of catalyst generating material, which describes carburization of metal at a contact with gas. Thus there were considered questions of influence of motion of gas stream on the process of carburization. Description contains physical and mathematical model of the microscopic system.

A physical model illustrates the microscopic process of carburization in $\tilde{N}\hat{I} - \acute{I}_2$-atmosphere. There are accepted, that in a solid body a fundamental process is diffusive, and in a gas phase, besides diffusion, there is convection. Studied gas atmosphere $\tilde{N}\hat{I} - \acute{I}_2$ and reactions $2\tilde{N}\hat{I} \Rightarrow \tilde{N} + \tilde{N}\hat{I}_2$, $\tilde{N}\hat{I} + \acute{I}_2 \Rightarrow \tilde{N} + \acute{I}_2\hat{I}$ provide the transmission of carbon to the solid.

Transporting of monoxide of carbon is arrived at by diffusion and convection. The area of contact consists of boundary layer of gas and solid the thickness of which is determined by different physical processes. Within the limits of pin area existence of three processes is possible: transmission of component in a gas phase, to the reaction on the border of division of phases and transmission of component in a solid body.

In a mathematical model basic equations in the partials of diffusive are presented and convective processes, what be going on at co-operation in a gas and hard phase.

In the beginning there are created a geometrical model, maximally close to the real terms. As catalyst generating materials there are used dispersible easy reducible oxides with the high concentration of defects in the initial state.

The nucleuses of new phase are formed on active centers which can serve superficial defects associates, clusters, wedging of distributions surface crystal etc. The structure for grates of graphite and carbide Fe_3C substantially differs from a grate α-*Fe*. Therefore a new phase at carburization of iron can be formed out of volume of initial phase, and diffusion of carbon in its is possible on point and lengthy defects.

Macromechanism of carburization for iron is based on supposition, that on all stages of process by place of reacting it is serves the border of division of initial hard phase (α-*Fe*) and gas phase (*CO*) and formation of new phase is possible in places with the least potential energy (superficial defects, defects of crystalline grate, wedging out of distributions).

Physical properties of matters, border terms, the generation of grid of eventual elements was set by the program in corresponding menus.

On the basis of analysis of the got results It is possible to conclude, that forming of carbon containing phase is begun with the surface of catalyst, to what the increased concentration of carbon testifies in its superficial layer, which diminishes on the depth of hard layer of catalyst. Change of concentration of carbon monoxide of in gas on motion co-operation not so meaningfully. However, in the places of superficial defects, i. e. in the places of the potential forming of new phase, there is depletion of gas mixture by the carbon monoxide that testifies on involving of the last in a process co-operating with a metallic phase.