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SOLVING ISSUES OF ENVIRONMENTAL SAFETY USING THE PROPOSED THREE-LEVEL MODEL OF CATALYTIC GAS NEUTRALIZATION

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Catalytic neutralization of organic gas compounds, carbon oxides and nitrogen is one of the most promising methods of conversion of harmful impurities. This method enables to process multicomponent gases with small initial concentrations of substances, to achieve high purification rates, to conduct the process continuously, to avoid in most cases the formation of secondary pollutants.

A three level mathematical model is proposed for heat release and the variation of the composition of a multicomponent gas mixture on the solid surface of a catalyst. The model contains three levels of description. The first describes the kinetics of a surface catalytic reaction. The second describes heat and mass transfer in the boundary layers. The third presents hydrodynamic and thermal models for the velocity of a multicomponent gas flow and the variation of temperature in the catalyst lattice.

The problems of increasing the efficiency of a heterogeneous catalytic process in a complex system that reflects the space of the neutralizer of harmful impurities of exhaust gases are given in this article.

The development of effective converters of harmful gas impurities is based on the need to create hydrodynamic and kinetic models for neutralization of exhaust gases, which take into account both the characteristics of the catalytic monolith construction and the multicomponent gas mixture of the exhaust gases.

Thus, a new three-level block model of the heterogeneously catalytic technology for neutralization of exhaust gases is proposed. The model is built on a hierarchical principle and includes several levels of description, corresponding to a certain space-time scale. The model defines all the main relationships between the processes occurring in the reaction at the micro-, mezo-, and macro levels. The block model is a kind of minimal model for an adequate description of the reaction in the catalyst layer. Each level can be detailed, taking into account additional factors and naturally integrating them into the full model, otherwise, to study certain approximations of the full model.

The proposed model was studied using the example of the CO oxidation reaction on the catalyst surface.

$$O_2 + 2* \underset{k_1^-}{\overset{k_1^+}{\Leftrightarrow}} 2[O]$$

$$CO + * \underset{k_2^-}{\overset{k_2^+}{\Leftrightarrow}} [CO]$$

$$[CO] + [O] \overset{k_3}{\Rightarrow} 2* + CO_2$$

$$\underline{CO + [O] \overset{k_4}{\Rightarrow} * + CO_2}$$

$$O_2 + 2CO \Leftrightarrow 2CO_2$$

The main distinguishing feature of the new model is the simultaneous consideration of all the basic physicochemical processes occurring during the reaction in the catalyst bed: reactions on the metal surface; internal diffusion in the pores of the catalyst grains; limited reagent feed rate; the thermal effect of the reaction; heat and mass transfer through the layer. The original numerical algorithm is also given, which allows to provide calculations on the full model.