Mathematical modeling of mass-heat transfer processes on the grain of a catalytic cracking catalyst

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Abstract. One of the most important processes ensuring deep oil refining both abroad and in Russia is the catalytic cracking process. This is the largest tonnage process of secondary oil refining and takes the second place in terms of the volume of processed raw materials after its primary distillation. The study of processes on the catalyst grain is necessary to create effective catalytic systems. The calculations of the chemical process on the catalyst grain are carried out on the basis of solving the equations of the mass balances of components and heat.

1. Introduction
When using a heterogeneous catalyst, the processes of mass and heat transfer can have a significant effect and the efficiency of a catalytic reactor with a heterogeneous catalyst is determined by both the thermodynamics and kinetics of the chemical reaction, and the processes of mass and heat transfer. In laboratory experiments, conditions are used in which mass and heat transfer can be neglected, for example, fine catalyst grains and high flow rates. But this cannot be done in an industrial reactor. Therefore, it is necessary to take into account the processes of heat and mass transfer in the catalyst grain and in the surface layer of gas or liquid. The heterogeneous-catalytic process on the catalyst grain includes the following stages: 1) reagent transport to the outer surface of the catalyst, 2) reagent transport to the inner surface of the catalyst, 3) adsorption of the reagent and reaction on the surface; desorption of products from the surface; 4) reverse transport of products from the inner and outer surfaces.

As a result of a chemical reaction with insufficiently intense diffusion, the concentration of the reagent in the catalyst grain decreases. The concentration in the center of the grain is lower than on the surface. If the stream is not sufficiently intensively washing the catalyst grain, then the reagent molecules diffuse weakly to the surface of the catalyst and their concentration on the outer surface is lower than the concentration in the stream. Therefore, it is necessary to take into account not only the change in the concentration of the substance as a result of the reaction and the diffusion of molecules in the pores of the catalyst, but also the diffusion of the substance through a thin surface layer (external diffusion) around the catalyst particle.

In addition, as a result of a chemical reaction, heat is generated in the catalyst grain, the temperature in the grain rises, and the reaction rate may increase (according to the Arrhenius law).
Through thermal conductivity, heat is transferred to the surface of the catalyst. If the thermal conductivity of the grain is small, then the temperature in the center of the grain may be higher than on the surface of the grain. If the stream does not wash the catalyst grain sufficiently intensively, then the surface temperature may be higher than the temperature in the stream. Therefore, it is necessary to take into account the heat release or absorption of heat as a result of a chemical reaction, heat transfer through heat conduction, heat exchange between the grain surface and the flow (external heat transfer). [1-5] The course of a chemical reaction with a change in the number of moles of the reaction and, accordingly, a change in the volume of the gas phase can lead to the formation of a hydrodynamic Stefan stream in the direction in which the number of moles of reactants decreases (to the center of the grain, if the reaction proceeds with a decrease in the number of moles, and from the center - with an increase in the number of moles). The Stefan flow also arises due to the difference in diffusion coefficients of different reagents [6].

2. The mathematical description of the catalytic process in the grain of the catalyst

Due to the fact that the shape and size of internal formations are usually not the same, each catalyst grain will have its own detailed structure and a corresponding description of the reaction. However, since individual internal formations are from nanometer to micrometer in size, and one catalyst grain is from one millimeter to one centimeter, one catalyst grain contains $10^9 - 10^{14}$ smaller particles. General statistical approaches can be applied to such a system and the catalyst grain can be considered as a homogeneous medium in which the reaction proceeds at a rate of mol / (m$^3$ grain · s), and the mechanism of matter and heat transfer is described within the framework of the diffusion mechanism.

Mass transfer processes in grain are generally described by the Stefan-Maxwell equations for each substance. When considering the catalyst grain as a homogeneous medium (quasi-homogeneous model), it is assumed that the temperature exchange between the gas in the pores of the grain and the solid phase of the porous medium proceeds intensively. Then the temperature $T$ of the solid phase of the porous medium and gas at each point of the grain can be considered the same and the heat transfer through the solid phase of the porous medium and gas at each point of the grain can be considered the same and the heat transfer process in the catalyst grain can be described by the well-known heat equation. Having made a series of approximations, we pass to the spherical coordinates. In these coordinates, the equations for the concentration of the $i$th gas component and for the temperature on an individual porous catalyst grain have the form:

$$r^2 \frac{\partial \omega_i}{\partial t} = \frac{\partial}{\partial r} \left( D_{ei} r^2 \frac{\partial \omega_i}{\partial r} \right) + \frac{r^2 R_i}{\rho}, i = 1, 2, ..., N$$  \hspace{1cm} (1)

$$\frac{\partial T}{\partial t} = \frac{1}{C_c} \left( \frac{r^2 \partial T}{\partial r} \right) + r^2 \sum_{j=1}^{Nr} Q_j W_j$$  \hspace{1cm} (2)

boundary conditions:

$$r = R_p:$$  \hspace{1cm} (3)

$$D_{ei} R_p^2 \frac{\partial \omega_i}{\partial r} = R_p^2 \beta_i (\omega_i^0 - \omega_i)$$

$$\lambda_e R_p^2 \frac{\partial T}{\partial r} = R_p^2 \alpha (T^0 - T)$$

$$\frac{d \omega_i}{d r} = 0:$$

$$\frac{d T}{d r} = 0$$  \hspace{1cm} (4)

where $C_c$ is the heat capacity of the catalyst grain, J / (m$^3$ grain · K), $\lambda_e$ is the effective thermal conductivity coefficient of the catalyst grain, J / (m · s · K), $\beta_i$ is the reaction number, $Q_j$ is the thermal effect of the $j$th reaction, J / mol, $W_j$ - molar speed of the $j$th reaction, i.e., here the velocity dimension has the form mol / (m$^3$ grain · s), $T$ - temperature, K, $\rho$ is the density of the gas mixture, g / m$^3$, $\omega_i$ is the mass fraction of the $i$th substance, the $i$th substance / mixture, t is the time, s, the $D_{ei}$ is the effective diffusion coefficient of the $i$th substance in a porous medium, m$^2$ / s, $R_i$ is the mass formation / expenditure rate i- component in a unit volume of the granule, i.e., here the velocity
dimension has the form of the $i$th substance / (m$^3$ grain • s), $R_p$ is the radius of the catalyst grain, m, $T^0$ temperature in the stream, K, $\omega_i^0$ is the mass fraction of the $i$-th substance in the flow, the $g$-th substance / gas mixture, $\beta_i$ is the mass transfer coefficient between the grain surface and the flow, m / s, $\alpha$ is the heat transfer coefficient between the grain surface and current, J / (m$^2$ • s • K) [7-8].

3. Results and Conclusion
Using the mathematical model (1), (2) with boundary conditions (3), (4), calculations were performed for the grain of the catalytic cracking catalyst. The six-component kinetic model with five reactions was taken as the basis [9]. A one-dimensional dependence of the concentration and temperature on the radius at a certain time was obtained in the form of a surface on the plane of the section of a granule passing through its center.

![Figure 1. Graph of concentration (vacuum gas oil) versus r.](image1)

![Figure 2. Graph of temperature versus r.](image2)

3. References
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