





The raw material from the balloon 2 through the rotameter (4) is fed to the reactor (diameter of reactor -34.2 mm; depth of reaction zone - 931 mm). The catalysts (15) with diameter of pellets 3.2 mm in amount of 270 cm<sup>3</sup> with a height of layer 437 mm are loaded to the reactor (1). Fillings (Raschig rings) have been backfilled on the catalyst layer a 64 mm high (17) and under the catalyst layer 136 mm high (16). Fillings (17) on the catalyst layer are filled with the aim of heating the feed zone to the temperature of 320°C.

The fillings (16), which are loaded into the reactor below the catalyst layer is required with the aim of to equalize the pressure on the cross-section of reactor that will evenly distribute the raw material at the reactor section. The reactor has been isolated with glass wool (18) and heated by a nichrome winding (20). The temperature inside of reaction zone and in isolation layer is controlled by thermocouples (13) and (14). The pressure of raw materials is controlled by the monometer (3). As the reaction temperature in the catalyst zone decreased to 280°C.

The waste gases from reaction zone come to the cooler (9). Liquid reaction products (including the condensed water, which is used for desorbing hydrocarbons from the catalyst surface) are cooled by running water and collected in the reservoir (10) but not condensed reaction products enter into the container (11) cooled by dry ice (12).

For the purpose of a desorption of the reaction products from the catalyst surface the steam is entered on the catalyst layer (15). For this purpose the spout (8) and pump (7) have been provided which supplies water from the dispenser to the reaction zone of the catalyst (15). Previously water evaporates in the filling region (17) and the steam with a temperature of 350-400°C is feed to the catalyst bed. Thus, from

the catalyst surface boiling hydrocarbons are desorbed which after passing a cooler (9) is condensed in the receiving tank 10 and 11. After desorption of boiling hydrocarbons at a temperature of 200-400°C the regeneration of oxidizing catalyst is carried out in the presence of air oxygen, which is fed from the balloon (5), having a pressure gauge (19). After regeneration, the reactor is purged with an inert gas in order to release of reactionary volume from air oxygen to its absence in the exhaust gases.

## Results and Discussion

The model of industrial reactor calculated taking into account the hydrodynamic mode allows to predict with high accuracy carrying out the studied system at change of the technological regime or composition of raw materials.

The plug flow reactor (PFR) is carried in laminar hydrodynamic regime. In such reactors, the reactants stream flows in one direction longwise of the reactor without hashing.

Hydrodynamic regime in PFR is characterized by the fact that any particle of stream moves in one direction longwise of reactor, the reverse (longitudinal) hashing absent. There is also no hashing on reactor section. It is assumed that the distribution of substances on this section is uniform, i.e., values of parameters of reaction mixture are identical. Each element of volume reaction mass  $dV_r$  moves along the length of the reactor without mixing up with the previous elements of the volume, and behaves as a piston in the cylinder, foxing out everything that is before it. Therefore, such driving mode of reagents is sometimes called piston or full displacement mode. The composition of each volume element sequentially changes longwise the reactor, as a result of the chemical reaction. So, for example, concentration of initial reagent varies progressively longwise the reactor from initial ( $C_{A0}$ ) to a final value ( $C_A$ ). The consequence of this movement mode of the reaction mixture is the fact that the residence time of each particle in the reactor is same.

For the mathematical description of the fixed bed catalyst there have been used quasi-homogeneous model of a layer of the granular catalyst. According to this model, the catalyst layer is presented in the form of a permeable solid medium through which a gas stream flows, and the chemical reaction proceeds with a speed equal to the observed speed of conversion. In this case, the catalyst layer is considered as a homogeneous medium with a continuous distribution of concentration, temperature, pressure and a flow rate.

Reaction rates are averaged by the volume of the layer, but the heat and mass transfer is determined by the effective thermal conductivities and diffusions coefficients, which depend on physical properties of the mixture, a flow rate, grain sizes, shape and the structure of a granular layer. In the adiabatic catalyst bed there is no radial heat-mass transfer. Heat transfer inside of grains takes place, mainly through a solid catalyst bulk which volume heat conductivity on several orders is higher than the thermal conductivity of gas.

As the length of the catalyst layer in industrial reactors is usually large enough, then the effect of axial diffusion is insignificant. While the Reynolds number above 100 heat and mass transfer occurs due to turbulent diffusion. In these conditions, the molecular diffusion can be neglected and the hydrodynamic regime approaches a plug flow regime [14].

There have been studied the influence of the temperature and rate of volume flow of supply of raw materials on liquid yield reaction, there have been installed the mechanism of the process. There have been compiled the kinetic equations describing the process of alkylation of C<sub>3</sub>-C<sub>4</sub> paraffins by olefinic hydrocarbons.



$k_i$	260°C	300°C	420°C	$E_i$ cal/mol	$K_{oi}$
$k_1$ $c^{-1}$	0.001545	0.00254	0.008027	7556.7	$0.194 \cdot 10^1$
$k_2$ l/mol·s	0.0151	0.0352	0.2465	12803.5	$0.269 \cdot 10^1$
$k_3$ l/mol·s	1.1	1.76	5.22	7145.3	$0.937 \cdot 10^0$
$k_4$ $c^{-1}$	0.000022	0.000063	0.000693	15767.9	$0.652 \cdot 10^2$
$k_5$ $c^{-1}$	0.0000128	0.0000211	0.00006675	7579.2	$0.164 \cdot 10^{-2}$
$k_6$ $c^{-1}$	0.0000159	0.0000408	0.0003554	14226.7	$0.109 \cdot 10^1$
$k_7$ l/mol·s	0.296	0.455	1.23	6542.5	$0.1426 \cdot 10^0$
$k_8$ l/mol·s	0.0109	0.0249	0.167	12523.6	$0.149 \cdot 10^1$
$k_9$ l/mol·s	0.348	0.68	3.197	10145.7	$0.518 \cdot 10^1$
$k_{10}$ l/mol·s	22.9	60.6	571.5	14754.2	$0.257 \cdot 10^5$
$k_{11}$ l/mol·s	4.26	7.58	28.6	8725.7	$0.161 \cdot 10^2$
$k_{12}$ l/l/mol·s	1.17	1.845	5.27	6907.6	$0.796 \cdot 10^0$
$k_{13}$ $s^{-1}$	0.00567	0.00844	0.0210	6014.1	$0.166 \cdot 10^1$
$k_{14}$ $s^{-1}$	0.00001128	0.0000168	0.000042	6044.26	$0.34 \cdot 10^{-2}$
$k_{15}$ l/mol·s	2.42	4.22	15.2	8427.4	$0.69 \cdot 10^1$
$k_{16}$ l/mol·s	894.0	1327.0	3295.0	5980.2	$0.253 \cdot 10^3$
$k_{17}$ l/mol·s	1.156	2.89	23.9	13906	$0.582 \cdot 10^3$
$n_1=0.937; n_2=0.817; n_3=0.91; n_4=0.77; n_5=0.98; n_6=0.87; n_7=0.99; n_8=0.93; n_9=0.99$					
The value of the adsorption constant $k_i^{ads}$				$Q_i$ heat of formation cal/mol	
$k_1^{ads}$	1.359	1.14	0.76	-2658.7	$0.11 \cdot 10^0$
$k_2^{ads}$	1.33	1.16	0.848	-2063	$0.189 \cdot 10^0$
$k_4^{ads}$	1.269	1.099	0.79	-2174.5	$0.163 \cdot 10^0$
$k_5^{ads}$	0.533	0.364	0.151	-5784.3	$0.226 \cdot 10^{-2}$
$k_6^{ads}$	0.956	0.864	0.684	-1541.3	$0.223 \cdot 10^0$
$k_7^{ads}$	0.937	0.768	0.486	-3010.5	$0.546 \cdot 10^{-1}$
$k_8^{ads}$	0.9	0.459	0.09587	-10309.3	$0.537 \cdot 10^{-4}$
$k_9^{ads}$	0.6934	0.387	0.1009	-8838.2	$0.1647 \cdot 10^{-3}$

Table 1: Kinetic parameters of the process of producing liquid products from a catalytic cracking gas.

$C_3H_8 \xrightleftharpoons[k_2]{k_1} C_3H_6 + H_2$	I	$n.C_4H_{10} + i.C_4H_8 \xrightarrow{k_{10}} C_8H_{18}$	IX
$i.C_5H_{12} + C_3H_6 \xrightarrow{k_3} C_8H_{14}$	II	$i.C_4H_{10} + n.C_4H_8 \xrightarrow{k_{11}} C_8H_{18}$	X
$i.C_4H_{10} \xrightarrow{k_4} i.C_4H_8 + H_2$	III	$n.C_4H_{10} + n.C_4H_8 \xrightarrow{k_{12}} C_8H_{18}$	XI
$n.C_4H_{10} \xrightarrow{k_5} n.C_4H_8 + H_2$	IV	$i.C_5H_{12} \xrightarrow{k_{13}} CH_4 + i.C_4H_8$	XI I
$i.C_4H_{10} \xrightarrow{k_6} 2C_2H_4 + H_2$	V	$i.C_4H_8 \xrightarrow{k_{14}} n.C_4H_8$	XI II

Routes, in which are formed connections with same chemical formula but different structure have been combined.

Comparison between the diffusion contribution values and the contribution of chemical reaction to change of reactants concentration in the grain with a diameter of 20 mm indicates that the internal diffusion of reactants proceeds much faster than chemical reactions.

#### 1. Diffusion of $C_3H_6$ and

$$i. C_4H_{10} = \frac{0.163 \cdot 10^{-4}}{0.001} \cdot 12.56 \times 10^{-6} \square 4.5 \times 10^{-7} \cdot 7.52 \times 10^3 \times 41.8 \times 10^{-10} \cdot 0.22216 \square 0.0000141451$$

#### 2. Diffusion $C_4H_8$ and i.

$$C_4H_{10} = \frac{0.137 \cdot 10^{-4}}{0.001} \cdot 12.56 \times 10^{-3} \square 7.58 \times 10^{-6} \cdot 7.52 \times 10^3 \times 41.8 \times 10^{-10} \cdot 0.172072 \square 0.00023826$$

#### 3. Diffusion of $C_3H_6$ and

$C_3H_8$  = From the above it follows that the rate of chemical reaction is not inhibited by the rate of diffusion of  $C_3$ - $C_4$  hydrocarbons to the inside of the catalyst grains.

### Conclusions

As a result of studies established that the alkylation process takes place in a plug flow reactor. The ratio of the thermal criteria of Peclet to the diffusion is within the 0.9-1.22. There have been provided a comparison of the values of contribution of diffusion and chemical reactions while changing of concentration of reactants in catalyst grain. At the same time, it has been found that the inner diffusion of reactants proceeds much faster than a chemical reaction.

It has been established that the internal diffusion of reagents proceeds much faster than the chemical reaction, so for  $C_4H_8$  and  $C_4H_{10}$

is within  $0.172072 \gg 0$ , 00023826. The ratio of thermal Peclet criterion ( $Pe_T$ ) to diffusion ( $Pe_D$ ) is in the range 0,91-1,22 that characterizes the process conditions in the reactor in an ideal displacement mode. There have been determined the values of the activation energy and the rate of constants of the principal reactions that occur in an industrial zeolite catalyst OMNICAT-210P. It means that the rate of chemical reaction is not inhibited by the diffusion of hydrocarbon inside the catalyst grains.

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