Table 1. Calculation results

Feed stream	Specific exergy, kJ/kg				
	TC-I	TC-II	TC-III	TC-IV	TC-V
Gasoline fraction	179.75	237.14	56.23	55.86	41.95
Diesel fraction	188.27	242.02	263.09	153.34	81.72
Residue	196.87	252.67	469.61	677.23	142.37

(TC-I);
- Two column Petlyuk scheme (TC-II);
- Two column direct sequence scheme (TC-III);
- Two column indirect sequence scheme (TC-IV);
- Two column scheme with distributed distillation and partial heat and material flow integration (TC-V);

For this task to be done the following calculations of specific chemical (ex_C) and physical (ex_P) exergy were carried out:

$$ex_C = l_{rev.}^L + l_{rev.}^S + l_{rev.}^G \quad (1)$$

$$ex_P = ex_T + ex_M \quad (2)$$

$l_{rev.}^L$ – exergy of reversal transferring from liquid to vapor, $l_{rev.}^S$ – exergy of reversal steam transferring to ideal state, $l_{rev.}^G$ – exergy of reversal gas mixture separation work (only for initial oil), ex_P, ex_M – isobaric (thermal) and isothermal (mechanical) parts of physical exergy.

Based on the obtained results we could make it possible to compare energy demands and estimate energy potential of outflows. The calculations let us to choose the most optimal scheme as well as suggest options of heat recuperation.

IMPROVING THE BENZENE ALKYLATION CATALYST PERFORMANCE WITH USE OF COMPUTER MODELING SYSTEM

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Linear alkylbenzene is one of the most common organic feedstocks used in the detergent industry. Linear alkylbenzene sulfonic acids of high molecular weight (245–260) are the anionic surfactants more used in all ranges of household detergents formulation, but especially in heavy duty laundry products, sometimes in combination with nonionics alcohol sulfates from tallow and soap. The ASA technology has almost completely replaced the older technologies for surfactants production due to improved biodegradability and cost-effectiveness. The technology of choice today is dehydrogenation of n-alkanes to n-alkenes followed by benzene alkylation to produce LAB and its further sulphonation.

Our previous researches were devoted to developing of mathematical models for all stages of the ASA manufacturing with due consideration of raw materials composition and links between the apparatuses. According to the above, we proposed to calculate the optimal flow of the HF alkylation catalyst to regeneration taking its current activity into account.

This includes following consequent stages:
- calculating the amount of dienes produced in

Table 1. Optimal values of HF flow rate to regeneration

HF optimal activity	Amount of heavy aromatics accumulated in the alkylation reactor, kg/h	Required HF flow rate to regeneration, m³/h
0.50	23.0	4.1
0.51	23.5	4.2
0.52	240	4.3
0.53	24.5	4.3
0.54	25.0	4.4
0.55	25.5	4.5
0.56	26.0	4.5
0.57	26.5	4.6
0.58	27.0	4.6
0.59	27.5	4.7
0.60	28.0	4.7

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the dehydrogenation reactor;

- calculating the amount of dienes supplied to the alkylation reactor;
- calculating the amount of heavy aromatics formed in the alkylation reactor at current HF activity;
- calculating the flow rate of HF to regeneration required to maintain the optimal catalyst activity providing the maximum LAB yield.

According to this methodology, we calculate the HF flow rate to regeneration assuming that the average content of heavy alkylaromatics in HF is 0.058 wt. %:

$$V_{HF_{per.}} = \frac{G_{HARreactor}}{0.0058 \cdot \rho_{HF}} \quad (1)$$

where $V_{HF_{per}}$ – required HF flow rate to regeneration, m³/h; $G_{HARreactor}$ – amount of heavy aromatics accumulated in the alkylation reactor, kg/h; ρ_{HF} – density of HF, kg/m³.

The required flow rate of HF to regeneration depending on the amount of heavy aromatics accumulated in the alkylation reactor is presented in Tab. 1.

Thus, amount of HAR accumulated in the alkylation reactor at current catalyst activity and HF required flow rate to regeneration is determined by amount of dienes formed in the dehydrogenation reactor.

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GAS-PHASE CATALYTIC OXIDATION OF 4-METHYLPYRIDINE

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Introduction

Isonicotinic acid (INA) and its derivatives have broad application as antitubercular drugs and stimulators of growth and maturing of many crops. INA is received by liquid-phase oxidation of 4-methylpyridine (4-MP) and its methylol derivatives of nitric acid [1]. Gas-phase catalytic oxidation of 4-MP by oxygen air on the oxide catalysts is the most effective method of obtaining pyridine-4-aldehyde and INA in one stage.

We tested the catalysts containing V_2O_5, SnO_2 and TiO_2 in the liquid-phase oxidation of 4-MP. The experimental results were interpreted by the quantum chemical computation. We studied the influence of oxide-modifiers on the nucleophilic properties of vanadyl oxygen and also on the deprotonation enthalpy of methyl group of chemisorbed substrate.

Experimental

The catalysts with different content of V_2O_5 and oxide-modifiers SnO_2 and TiO_2 were prepared by mixing the initial oxides in the required molar ratio. The obtained oxide mixture was carefully milled and pressed in the form of tablets which then calcined in an air flow at 600 °C for 2 h.

The catalytic tests were conducted in the flow-circulating fixed bed reactor with a reaction tube from stainless steel with a 20-mm inner diameter and a 120-cm length. The reaction tube was placed inside an electric oven. 100 ml of the catalyst fraction 3–5 mm was used in the experiments. Delivery rate of 4-MP was 37.5 g/hour on 1 liter of the catalyst and a molar ratio Substrate : O_2(air) : $H_2O = 1 : 14 : 110$.

The products of the reaction were caught in the air lift type scrubbers irrigated by water and