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### **Modeling of organizational structures of enterprises of Tatarstan oil and gas-chemical complex**

*Keywords:* shared profit sharing, resource saving, production organization, oil and gas chemical complex, innovations.

*Abstract.* The article is devoted to the actual topic of modeling organizational structures of enterprises of the oil and gas chemical complex, which allow to increase the competitiveness of products, by increasing energy and resource saving, minimizing the formation of the company's waste. The purpose of the article is to simulate the management of petrochemical enterprises aimed at increasing the efficiency of enterprises, using innovative energy and resource-saving technologies. The leading method to investigate this problem is the modeling method, which allows us to consider this problem as a purposeful and organized process to improve the management of oil and gas chemical enterprises. The results of the research make it possible to regulate the innovative activity of petrochemical enterprises in a better and more targeted way through the use of innovative forms of management and can be used in the framework of sectoral programs, they are of interest to state statistics bodies and ministries and agencies responsible for strategic analysis and planning.

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### **ACCENT of the ISSUE: Petrochemicals in Azerbaijan**

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### **Investigation of physico-chemical properties of monoalkyl(C<sub>8</sub>-C<sub>12</sub>)phenolformaldehyde oligomers, modified by means of imidazolines and amidoamines based on natural petroleum acids and polyamines**

*Keywords:* monoalkyl(C<sub>8</sub>-C<sub>12</sub>)phenolformaldehyde oligomers, physico-chemical properties, imidazolines, amidoamines, distilled petroleum acids, polyamines.

*Abstract.* The relevance of research towards the synthesis of oligomers based on phenol and its derivatives with formaldehyde is associated with both the availability of raw materials, and the possibility of chemical modification and the extensive use of them in various sectors of the economy. The starting components for the synthesis of phenol-formaldehyde oligomers (FFO) can be prepared from both oil and gas, or from coal, which reserves are inexhaustible. Among the areas of application the special place is occupied by the paint industry, obtaining film-forming substances anticorrosion additives, which is due to the presence of FFO functional groups and fragments defining their protective properties. The latter include hydroxyl, methylol groups, and a delocalized p-electron cloud of phenolic nuclei which provide effective adhesion to the metal surface exhibiting protective properties. Modification with nitrogen compounds favors this by introduction of polar functional groups containing nitrogen - one of the electronegative elements.

There are some works, where amines, amides, triazines, amino acids, amino alcohols, etc. were used as FFO modifiers, whereby products with valuable properties were obtained. In this article we proposed to modify imidazolines and amidoamines based on natural oil distilled acids (DPNK) and polyamines (PA) – diethylenetriamine (DETA), triethylenetetraamina (TETA), polyethylene polyamine (PEPA) [11]. To achieve good solubility in non-polar solvents alkylphenols with C<sub>8</sub>-C<sub>12</sub> alkyl groups in the para – position were used as the phenolic component. Modification by monoalkyl (C<sub>8</sub>-C<sub>12</sub>)amidoamines and imidazolines FFO based on DPNK and PA was held by reacting a phenolic component with formaldehyde in a molar ratio of 1 : 0.85, temperature 98-100°C for about 3.5-4 hours until the turbidity, pointing at formation of condensation centers and oligomeric chain, followed by addition of a nitrogen-containing compound in parts at low temperature (≈50-55°C) and raising the temperature up to 98-100°C at which the process was carried out for hour more. The final product is a resinous, light or dark brown, also lurid mass.

The physico-chemical properties of monoalkyl(C<sub>8</sub>-C<sub>12</sub>)phenolformaldehyde oligomers, modified by imidazolines and amidoamines based on natural distilled oil acids and diethylenetriamine, triethylenetetraamine, polyethylenepolyamines have been investigated. The solubilities of the synthesized oligomers in various solvents of polar and non-polar nature have been determined. Study provides oligomers synthesized as corrosion inhibitors in the composition of mineral oils.

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### Conservative liquids on based the composition of dialkyldithiophosphates of metals and alkylamines

**Keywords:** dithiophosphates, phosphorsulfuration, corrosion inhibitors, conservative liquids.

**Abstract.** Metal complexes of O,O-dialkyldithiophosphates acids have been developed and studied. The using of these metal complexes as components of compositions with nitrogen-containing compounds are created conservative liquids. In gidrokamera, sea water and sulfuric acid medium (0,001% solution) the composition on the corrosion resistance have been tested.

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### Alkylation of *para*-cresol with isopren in the presence of phosphorus-containing catalyst

**Keywords:** *para*-cresol, cyclodimer of isoprene, catalyst,

2-[3(4)-methylcyclohexen-3-yl-isopropyl]-4-methylphenol.

**Abstract.** It was given the results of alkylation reaction of *para*-cresol with diprene, dipentene and mixture of them (160-180°C fractions) in the presence phosphorus-containing of catalyst. The effect of various parameters (temperature, duration of the reaction, mol ratio of reactants and amount of catalyst) to the yield of desired products was studied and for each reactions, optimal conditions were found. It was determined that, in optimal conditions the percentage yield of desired products was 71.5-77.3 % and selectivity was 93.8-95.2%.

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### Optimization of the esterification process of 2,3-dimethylbicyclo/2.2.1/hept-5-ena with aliphatic monocarbonicacids C<sub>5</sub>-C<sub>9</sub>

**Keywords:** esterification, bicyclic diol esters, lubricating oils, optimization, second-order equation.

**Abstract.** In this work, the influence of the input variables is studied: the reaction temperature, the molar ratio of dimethylbicyclo/2.2.1/hept-5-ene (DMBCH): caproic acid, the reaction time, the amount of catalyst to the yield of dicaproatabicyclo/2.2.1/hept-5-ene (DCBCH).

The work shows the experimental results obtained by studying the effect of the above input variables. It was found that, when the temperature is changed from 130 to 160°C, the yield of the desired product increases to a value of 85,2%. Subsequent increase in temperature leads to a decrease in the yield of DCBCH to 83%.

Mathematical processing of the experimental data made it possible to obtain the dependence of the yield of the target product on temperature in the form of a regression equation of the second order:  $Y_1 = -0,0135 \cdot X_1^2 + 4,49 \cdot X_1 - 287,36$ .

When studying the effect of the molar ratio of DMBCH: caproic acid, it was found that the ratio from 1:1 to 1:2,5, the yield of the desired product increased to 86,4%. When the molar ratio is increased, the yield is reduced to 84%. Mathematical processing of experimental data to find the dependence of the yield of the target product on the molar ratio in the form of a second-order regression equation:  $Y_2 = -10,73 \cdot X_2^2 + 66,3 \cdot X_2 - 11,16$ .

When investigating the effect of the reaction time on the yield of the desired product in the range of 1-3 hours, it was found that to 2 hours the yield increased and reached 85,6%. The further increase in the reaction time leads to a decrease. Mathematical processing of the experimental data made it possible to find the dependence of the yield of the target product on the duration of the reaction in the form of a regression equation of the second order:  $Y_3 = -17,4 \cdot X_3^2 + 85,7 \cdot X_3 - 18,2$ .

When studying the effect of the amount of catalyst on the yield of the desired product, it was found that with a catalyst amount of 1,5% by weight, the yield of the desired product reached a maximum value of 89,2%. A further increase in the amount of catalyst leads to a decrease in the yield of the desired product. The mathematical dependence of the yield of the desired product on the amount of catalyst describes the second-order equations:  $Y_4 = -39,2 \cdot X_4^2 + 116,84 \cdot X_4 + 4,9$ .

The particular dependences of  $Y_i$  from each factor  $X_i$  are approximated by second-order equations. To compose a generalized equation of the output optimization parameter, which takes into account the simultaneous influence of all input variables. It applies a probabilistic-deterministic method of experiment planning, found the dependence of the yield of the target product  $Y_i$  on all input variables  $X_i$  at the same time. The equation of the second order has the form:  $Y' = 32,76 - 0,359 \cdot X_1 + 0,455 \cdot X_1 X_2 + 0,496 \cdot X_1 X_3 + 0,72 \cdot X_1 X_4 - 0,00634 \cdot X_1^2 - 12,259 \cdot X_2^2 - 15,768 \cdot X_3^2 - 38,64 \cdot X_4^2$ .

Computer calculations yielded the maximum yield of the target product  $Y'=91,5\%$  of the mass, with a reaction temperature of  $170^{\circ}\text{C}$ , a molar ratio of the original components of 1: 3 mol/mol, a catalyst amount of 1,5% by mass and a reaction time of -1,5 hours.

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## **PETROLEUM PRODUCTS: technology, innovation, market**

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### **Investigation of the rheological properties and thermal-oxidative stability of solutions of polyisobutenes in petroleum and synthetic oils**

*Keywords:* industrial oil, mineral oil, synthetic oil, polyalphaolefins, thermooxidation stability, dynamic viscosity, polymer degradation, rate constant of chemical reaction, activation energy.

*Abstract.* Polyisobutylenes with different molecular mass are widely used as functional additives in lubricating materials, nevertheless rheological properties and oxi-thermal stability of polyisobutylene solutions in fossil and synthetic oils are rather poorly studied. In this article authors present the results of research of thickening ability of polyisobutylene with different molecular mass (85000-200000). The dependance of the dynamic viscosity upon the molecular mass of PIB and the nature of the dissolving medium is produced. The calculation of rate constant and activation energy of oxi-thermal destruction of PIB molecules in fossil and synthetic oils is presented. It has been shown that PIB has an increased oxi-thermal stability in fossil oil in comparison with polyalphaolefin oil.

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## **MATHEMATICAL SIMULATION**

*Kuvykin V.I., Bryukhanov M.V., Kuvykina E.V., Piskunov I.V., Sychev A.G.*

### **Improvement of viscosity calculation of heavy oil product mixes in production planning systems**

*Keywords:* viscosity, modeling, linear programming, refinery planning.

*Abstract.* It is shown that viscosity calculations of heavy oil product mixes, used in production planning mixes, should be revised. Results of calculations and experimental measurements of mixes viscosity are compared. A method to update coefficients of Walter's equation is proposed. This can improve accuracy of technological calculations and production planning, as well as reduce costs of oil products compounding. An economic assessment of formula parameters impact on the refinery profitability was carried out.

## **CONFERENCES. SEMINARS. EXHIBITIONS**

**The 7<sup>th</sup> summit of the heads of the oil and gas industry of Russia and CIS countries  
(21–22.06.2017, Sochi) / Post-release**

**The 22<sup>nd</sup> World petroleum Congress "Russia's energy Future" (9- 13.07.2017, Istanbul) / Post-release**

## **PORTRAITS**

**85<sup>th</sup> anniversary of birthday of V.P. Kovalenko is dedicated to**

## **MATERIALS of the PETROCHEMICAL and REFINERS ASSOCIATION**

**Extracts of the protocol #136 of ANN board meeting of 17.05.2017**

**Subject – Modernization and construction of new petrochemical plants**