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COMPARATIVE CHARACTERISTICS OF EXTRACTANTS FOR THE SEPARATION OF AROMATIC HYDROCARBONS

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Abstract. This article discusses methods for separating liquid mixtures through extraction, the types of solvents used, their physicochemical properties, and the factors influencing the selection of suitable solvents. The advantages and disadvantages of the extraction process are also analyzed.

Keywords: solution, extraction, raffinate, extract, extractant, selectivity, aromatic hydrocarbons, benzene.

Introduction.

The process of separating one or more components from a liquid mixture using selective solvents is known as liquid extraction. During the extraction process, when the liquid mixture is combined with a selective solvent, only the desired components from the initial mixture dissolve well in the solvent, while the remaining components either dissolve poorly or not at all. In industrial processes, the extraction method is used similarly to distillation to separate specific components from solutions. The choice of the extraction method from the above-mentioned options depends on the properties of the substances to be separated. In the distillation process, the separation of components from the mixture is typically achieved through heat, based on differences in their boiling points. In contrast, the extraction method does not require heat. Therefore, when the boiling points of the components in the initial mixture are close to each other, or if they are unstable at high temperatures, distillation processes are avoided, and extraction is preferred, based on the differing volatility of the components.

The extraction process occurs in the liquid phase. When a selective solvent is added to a hydrocarbon mixture, the mixture separates into two phases: raffinate and extract. The extract phase contains concentrated arenes. Solvents used to separate arenes from paraffins and naphthenes exhibit low solubility for non-aromatic compounds, high power for arenes, and high selectivity, causing the mixture to separate into two phases. To regenerate the solvent from the extract and raffinate phases, there must be a significant difference in the densities and boiling points of the solvent and the extracted substances.

An extractant is a substance that separates the desired component from a liquid mixture. The main requirements for solvents are as follows:

- Selective action with respect to the desired component.
- The ability of the solvent to dissolve and absorb the desired component.
- The possibility of easy and complete separation of the absorbed component from the solvent, i.e., re-extraction.
- Easy separation of the phases into distinct layers.
- Safety in handling, meaning the solvent should not be toxic, volatile, or have explosive properties.
- Stability during storage and use (in both extraction and re-extraction processes).
- Low cost.

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- Readily available, i.e., not rare.
- The solvent density must be lower than that of the extracted substance.

Research Methodology

When extracting high-purity aromatic hydrocarbons (99-99.9%) from various concentrates, it should be noted that arenes may form azeotropic mixtures with naphthenes and paraffins, whose boiling points are close. Azeotropic and extraction distillation, or selective extraction methods, are employed to separate the arenes.

In the extraction process, the following factors must be considered:

- The effect of temperature on the solvent's capacity and selectivity.
- The dependence of the solvent's selectivity on the concentration of arenes in the initial mixture.
- The relationship between solvent selectivity and the molecular mass of hydrocarbons within the same homologous series.
- The ratio of solvent and raw material quantities, as well as the recirculation ratio.

In the extraction process, solvents with selective properties–known as extractants – are used, which are chemical compounds or their mixtures capable of dissolving various substances. Examples of such solvents include water, alcohols, acids, alkalis, ethers, benzene, toluene, xylene, or their combinations. Solvents are classified based on their properties, such as volatility, viscosity, density, dielectric constant, or chemical reactivity. The chemical characteristics of solvents, particularly their toxicity or non-toxicity, are of primary importance. Standard solvents are categorized according to their acidic, basic, or amphoteric properties. Depending on the dissolved substance, a solvent can act as either an acid or a base. Water is considered an almost ideal amphoteric solvent. Solvents that act as bases relative to water are called acidic solvents, while those acting as acids relative to water are considered basic solvents. This classification takes into account the movement of electrons in functional groups that participate in solution formation. Accordingly, a solute molecule that donates an electron pair is designated as a basic (donor) solvent. Representatives of donor solvents include aniline, pyridine, dimethyl sulfoxide, and both simple and complex ethers. Solvents that accept an electron pair from the solute are referred to as acidic or acceptor solvents. These include carboxylic acids, phenols, acid chlorides, and fully halogenated aliphatic hydrocarbons such as chloroform and dichloroethane. Alcohols and ketones, in the absence of water, are considered amphoteric solvents. Hexane, carbon disulfide, and carbon tetrachloride are classified as "inert solvents."

One of the physical properties used in selecting solvents is their dielectric constant. Solvents are typically divided into those with low polarity (ranging from 2 to 12) and high polarity (above 50). For example, water has a dielectric constant of 78, whereas benzene's is only 2.3. Experimental data show that two oppositely charged particles or dipole molecules interact in water with nearly 80 times less energy than in a vacuum. In benzene, this interaction energy is reduced only about twofold. Therefore, water is classified as a highly polar solvent, along with other substances such as propylene carbonate, hydrazine, formamide, and sulfuric acid, which are close to water in polarity.

Due to its significant technical and economic advantages, the extraction process is widely used in industry. Multistage and counter-current extraction methods are implemented in column extractors and mixer-settler units (Figure 1).

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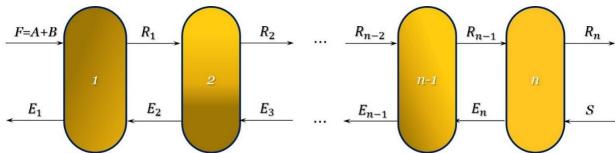


Figure 1. Scheme of Multistage and Counter-Current Extraction:

1, 2, 3, \cdots , n-1, n- stages;

 E_1 – extract exiting from the first stage;

 R_n – raffinate exiting from the last stage.

In recent years, industrial liquid extraction has widely adopted counter-current methods using reflux and employing two solvents.

Discussion and Results

Knowing the types and properties of solvents allows the implementation of various reactions. The use of solvents has solved the problem of separating aluminum at low temperatures during the electrolysis process. This approach has also enabled the production of aluminum-based protective and decorative coatings. Acetone, acetonitrile, benzene, diethyl ether, dimethylacetamide, dioxane, acetic acid, ethanol, formamide, methanol, nitrobenzene, pyridine, carbon tetrachloride, chloroform, ethyl acetate, cyclohexane, methyl ethyl ketone, octane, turpentine, carbon disulfide, tetralin, tributyl phosphate, and others are various solvents that play an important role in industry and the national economy.

For the extraction and rectification separation of aromatic hydrocarbons, solvents such as diethylene glycol (DEG), triethylene glycol (TEG), sulfolane, N-methylpyrrolidone, N-formylmorpholine, and other substances are widely used in industry (some of their physicochemical properties are presented in Table 1).

Table 1. Physicochemical Properties of Solvents

Parameters	DMSO	EG	DEG	TEG
Molecular weight	78,13	62,07	106,12	150,18
Refractive index, n_D^{20}	1,4785	1,4318	1,4468	1,4518
Density, ρ_4^{20}	1,1	1,1088	1,177	1,1274
Boiling point, °C	189	195	247	287
Freezing point, °C	+ 18,4	-69,0	-8,0	-5,0
Viscosity, sPz (25°C da)	2,0	19,9	31,84	-
Heat capacity, <i>kal/g</i> °C	0,49	0,219	0,57	0,43
Surface tension, <i>erg/sm</i> ² (25 °C da)	43,0	46,1	45,4	-
Dipole moment, debay	4,3	2,3	2,31	2,99
Heat of vaporization, kJ/mol	51,2	56,9	53,6	71,4

In the extraction process, the following factors must be taken into account:

- the effect of temperature on the solvent's capacity and selectivity;
- the dependence of solvent selectivity on the concentration of arenes in the feedstock;

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- the relationship between solvent selectivity and the molecular mass of hydrocarbons within the same homologous series;
- the quantities of solvent and feedstock, as well as the recirculation ratio.

When extracting high-purity aromatic hydrocarbons (99–99.9%) from various concentrates, it is important to consider the formation of azeotropic mixtures between arenes and naphthenes or paraffins with boiling points close to those of the arenes. To separate arenes, azeotropic and extractive distillation or selective extraction methods are employed.

Conclusion and Recommendations

Selective extraction is predominantly used in industrial equipment for the separation of aromatic hydrocarbons. In this process, mixtures of arenes are first separated and subsequently fractionated into benzene, toluene, and xylenes.

The selective extraction process is based on the limited solubility of certain components (arenes) or their preferential dissolution in the solvent compared to other components. Therefore, the correct choice of solvent is of critical importance. Analyzing the theoretical aspects of separating aromatic hydrocarbons from various fractions, examining the selective solvents used in the extraction process along with their advantages and disadvantages, and studying the main industrial extraction methods and their characteristics for obtaining aromatic hydrocarbons from different fractions, allows for the optimal selection of the type and ratio of extractants.

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