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to the dissertation written on the topic

Ionic liquids and deep eutectic solvents for cleaning motor fuels

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General job description. The research topic of using ionic liquids and deep eutectic solvents for refining motor fuels is very relevant in the context of sustainable energy and environmental protection. Motor fuels such as gasoline and diesel often contain additives such as sulfur, nitrogen, and aromatic hydrocarbons that contribute to air pollution and greenhouse gas emissions when burned. Reducing the emissions of these pollutants in the presence of ionic liquids and deep eutectic solvents, thereby reducing the environmental impact associated with motor fuel combustion.

Relevance of the research topic . Nitrogen dioxide (NO_2), sulfur dioxide (SO_2), and carbon monoxide are all significant ambient air pollutants. Controlled human exposure studies have shown that experimental exposures to SO_2 and NO_2 alter airway physiology. Given the disastrous effects of SO_2 on people and ecosystems, policymakers are introducing stricter regulations, mandating the use of low-sulfur gasoline. The European Union introduced the Euro-5 fuel standard in January 2009, which requires a maximum sulfur content of 10 ppm in both diesel and gasoline. Currently, the industry usually uses the process of hydrodesulfurization (HDS) of fuel oils, in which S-compounds undergo a chemical reaction with hydrogen in the presence of Co-Mo/Al_2O_3 catalysts, or Ni-Mo/Al_2O_3 are converted into hydrogen sulfide (H_2S) and subsequently removed from the fuel oil. for. oils. High pressure (~20 MPa) and high temperature (~400 °C) and an efficient and noble catalyst are required to achieve the appropriate level using HDS. There are two types of sulfur compounds: active sulfur compounds and inactive sulfur compounds. The main active sulfur compounds are elemental sulfur, hydrogen sulfide, and mercaptan, which can be removed industrially using hydrodesulfurization technology (HDS). Inactive sulfur compounds that are difficult to remove industrially include mainly thiophene, benzothiophene, dibenzothiophene and its derivatives. In addition, the removal of aromatic compounds from fuel was an important issue. This is because the presence of aromatic compounds in the fuel prevents the production of very low sulfur fuel.

The research topic of using ionic liquids and deep eutectic solvents for refining motor fuels is very relevant in the context of sustainable energy and environmental protection. Motor fuels such as gasoline and diesel often contain additives such as sulfur, nitrogen, and aromatic hydrocarbons that contribute to air pollution and greenhouse gas emissions when burned. Reducing the emissions of these pollutants in the presence of ionic liquids and deep eutectic solvents, thereby reducing the environmental impact associated with motor fuel combustion.

Ionic liquids and deep eutectic solvents are green alternative solvents to conventional organic solvents. They have unique properties such as low volatility, high thermal stability and tunable chemical characteristics. These solvents can be synthesized from renewable resources, making them more sustainable and reducing dependence on fossil fuel-derived solvents. Ionic liquids and deep eutectic solvents have special properties that allow targeted and selective removal of pollutants from motor fuels. This versatility makes them promising solvents for the development of effective cleaning processes that can remove certain impurities without affecting the desired fuel properties.

The purpose of the work: Synthesis of ionic liquids and deep eutectic solvents. Calculation of the ability of the obtained solvents to remove sulfur compounds and nitrogen compounds from motor fuel.

To achieve this goal, the following tasks were set:

– Synthesis of new ionic liquids and deep eutectic solvents effective for extraction and study of their physical and chemical properties;
– Evaluation of the flexibility of ionic liquids and deep betaine-based eutectic solvents (DESs) in the temperature range from 293.15 K to 323.15 K at atmospheric pressure;
– COSMO-RS (conductor-screening model for real solvent) screening model based on statistical thermodynamics and quantum chemistry to estimate the activity coefficients of mixture components;

Form of research *:* Ionic liquids and deep betaine-based eutectic solvents (DESs), namely 1-butyl-3-methylimidazolium chloride, 1-ethyl-3-methylimidazolium ethyl sulfate, betaine:glycerol [1:2], and betaine:ethylene glycol [1:3].

Field of study. Solving separation problems arising in the petroleum industry, liquid-liquid equilibrium (LLE) six ternary systems {thiophene + betaine: glycerol [1: 2] and betaine: ethylene glycol [1: 3] + n-heptane}, {pyridine + betaine: glycerol [1: 2] and betaine: ethylene glycol [1: 3] + n-heptane } and {toluene + betaine: glycerol [1:2] and betaine: ethylene glycol [1:3] + n-heptane} are used in systems .

Research area: Ionic liquids and deep eutectic solvents have unique chemical properties and provide promising opportunities for effective removal of pollutants from motor fuels. Research in this area covers a wide range of aspects, ranging from the development of optimal solution compositions to the study of mechanisms of interaction with various pollutants. An important part of this research area is also the assessment of the environmental and economic benefits of using these purification methods, as well as the integration of the developed technologies into industrial refining processes. Approaches based on ionic liquids and eutectic solvents are positioned as a promising solution to reduce the harmful effects of fuel emissions on the environment and improve the standards of purity and efficiency of motor fuels. This interaction with the oil industry not only supports innovative cleaning methods, but also affects the overall sustainability of the fuel industry in the face of rapid changes in environmental safety requirements and the sustainability of fuel production.

Scientific and technical level of research and metrological support of research work. Classical and modern physico-chemical research methods were used during the research work. Synthesis of given green solvents K. It was studied using physico-chemical methods in the laboratory of the Department of Chemical and Biochemical Engineering of Kazakh National Technical University named after Satbaev, Laboratory of Reactions and Technological Engineering, University of Lorraine (Nancy, France). In particular, the following methods of sample preparation and research were used:

- betaine:glycerol [1:2] and betaine:ethylene glycol [1:3] liquid-liquid equilibrium (LLE) six ternary systems {thiophene + betaine:glycerol [1:2] and betaine:ethylene glycol [1:3] + n-heptane}, {pyridine + betaine:glycerol [1:2] and betaine:ethylene glycol [1:3] + n-heptane} and {toluene + betaine:glycerol [1:2] and betaine:ethylene glycol [1: 3].
- the composition of samples was used for quantitative determination of organic compounds by gas chromatography (Perichrom 2100) equipped with FID detector.
- In this work, the phase diagrams were determined using COSMTherm software version C30. COSMO results for thiophene, toluene, pyridine, glycerol, and ethylene glycol were generated in the COSMTherm database. Betaine's COSMO files were generated using Gaussian 09 Revision D.01. Density functional theory (DFT) was performed at the BVP86/TZVP/DGA1 level of theory using a dense self-consistent field (SCF) for the convergence method and DGA1 for the fitting set.

Scientific novelty of the obtained experimental results

– For the first time, the COSMO-RS model, a liquid of six ternary systems consisting of the equilibrium liquid n-heptane, betaine:glycerol [1:2] or betaine:ethylene glycol [1:3] and thiophene or pyridine or toluene, was used to estimate the activity coefficients of components in mixtures.
– The mass ratio of solute distribution (β) and selectivity values (S) calculated on the basis of experimental data for the given systems showed that betaine:ethylene glycol [1:3] was more effective for removing pyridine or thiophene from aliphatic media.
– The NRTL model allowed us to represent the liquid-liquid equilibria in the six ternary systems studied in this work with good accuracy. Ternary systems containing thiophene and pyridine were proposed in the COSMO-RS model.
– First, deep eutectic solvents and ionic liquids with the highest degree of extraction were selected and their extractability efficiency was studied.

Practical significance of the work.

Sulfur and nitrogen compounds in motor fuels such as gasoline and diesel can contribute to air pollution when burned in engines. Many countries have strict regulations on the maximum permissible levels of these pollutants in fuel to reduce emissions and protect air quality. DES-based treatment helps meet these regulatory requirements by effectively removing these impurities. Sulfur and nitrogen compounds in motor fuel can cause harmful emissions such as sulfur dioxide (SO_x) and nitrogen oxides (NO_x) during combustion . These emissions are not only harmful to the environment, but can also reduce engine performance and performance. By treating fuels with DES, combustion efficiency can be improved and emissions can be reduced, which is especially important for meeting emission standards and improving fuel economy.

Sulfur and nitrogen compounds can poison catalytic converters in vehicles. These catalysts are critical to reducing harmful emissions, and their performance can deteriorate when exposed to impure fuels. DES-based cleaning helps protect these catalysts and extends their life, saving on maintenance and replacement costs. Clean fuels with reduced sulfur and nitrogen content lead to lower emissions of sulfur dioxide and nitrogen oxides, major contributors to acid rain and smog. Using DES to refine fuels contributes to a cleaner and healthier environment by reducing these harmful emissions. Removing impurities with DES can result in higher quality fuel with better combustion properties, which can lead to improved engine performance, reduced knocking and increased fuel efficiency.

Purification of sulfur and nitrogen compounds from motor fuels using deep eutectic solvents is of practical importance in complying with environmental protection regulations, increasing engine efficiency, protecting catalysts, reducing harmful emissions, extending engine service life, maintaining fuel stability, and increasing fuel quality and productivity. These advantages make DES-based refining an important step in the production of cleaner and more efficient motor fuels.

The main cases (principles) recommended for protection:

- In the first part of the work, 1-butyl-3-methylimidazolium chloride and 1-ethyl-3-methylimidazolium ethylsulfate ionic liquids were synthesized and their physical and chemical properties were studied accordingly. In addition, they were analyzed by NMR and IR spectrometer methods, and the extractive properties of the obtained solvents were determined;

- In the second part, the liquid-liquid phase equilibrium was studied at atmospheric pressure at a temperature of 298.15 K in the following ternary mixtures: {thiophene + n-heptane + betaine: glycerol [1: 2]}, {pyridine + n-heptane + betaine: glycerol [1:2]}, {toluene + n-heptane + betaine: glycerol [1: 2] }, {thiophene + n-heptane + betaine: ethylene glycol [1: 3]}, {pyridine + n-heptane + betaine: ethylene glycol [1: 3] } and {toluene + n-heptane + betaine:ethylene glycol [1:3]}.

- Compositions of equilibrium phases were determined by gas chromatography. Extraction efficiency was estimated as a result of calculation of diffusion coefficients and selectivity.

- Kinetic parameters, as well as temperature and mass relationships were studied to determine the optimal extraction conditions. Experimental data were compared using the NRTL and COSMO-RS models.

- Results of synthetic fuel extraction using selected ionic liquids and deep eutectic solvents are presented using one or three step extractions under optimal conditions.

Connection with the main scientific work plan

The proposed dissertation work was funded by the targeted funding of the

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Publication of the results in the press. The main results of the dissertation work are published in 10 co-authored publications, including 2 articles in international scientific publications included in the Scopus database; 2 articles in journals recommended by the Control Committee in the field of Education and Science of the Ministry of Education and Science of the Republic of Kazakhstan; published in 6 materials of international and national scientific conferences.