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THERMAM 2017

6th Rostocker International Conference:
"Thermophysical Properties
for
Technical Thermodynamics"

Institute of Technical Thermodynamics

University of Rostock,
Rostock, Germany

17 – 18 July, 2017

INSTITUTE OF TECHNICAL THERMODYNAMICS

THERMAM 2017

6th ROSTOCKER INTERNATIONAL CONFERENCE: “THERMOPHYSICAL PROPERTIES FOR TECHNICAL THERMODYNAMICS”

17 - 18 July 2017

University of Rostock
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2017

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Density measurements up to 4000 bar and temperatures up to 200 °C

Vapor pressure measurements at high temperatures

Density measurements at ambient pressure and various temperatures

Density measurements up to 1400 bar and temperatures up to 200 °C

Gas solubility measurements in liquids at high pressures and wide range of temperatures

Vapor pressure measurements at small temperatures

BOOK OF ABSTRACTS

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Preface

6th ROSTOCKER INTERNATIONAL CONFERENCE ON THERMOPHYSICAL PROPERTIES FOR TECHNICAL THERMODYNAMICS

Thermodynamics is a very fascinating scientific field which has to do with many different phenomena in nature and technique. As an interesting example we can regard climate change which at the moment is on the agenda of many political decision makers and scientists. Climate change is partly caused by the emission of the carbon dioxide molecule to the atmosphere from farming, from technical combustion in energy technique and transport and from many other human related processes. The heat transfer processes in the atmosphere clearly have to do with thermodynamics. On the other hand, measures to reduce human impact on the environment, like CCS, carbon capture and storage, from combustion also involve thermodynamics processes. To solve and handle thermodynamics problems one needs “Thermophysical and Mechanical Properties of Advanced Materials”. One example is the possible capture of carbon dioxide from atmosphere or exhaust gases in ionic liquids. To make this technically feasible data for the thermophysical property of solution of carbon dioxide in the advanced material of an ionic liquid are needed.

Within this conference we want to bring together international scientists and engineers who work in the very broad field of “Thermophysical and Mechanical Properties of Advanced Materials”. This is a very interesting and modern research field. It covers experimental and theoretical new results for thermophysical properties, new measurement techniques and their applications, molecular modeling with new theoretical insights, applications which show the improvement done with the described research for thermophysical properties and mechanical properties for materials like nanofluids, nanocomposites, alternative solvents, metals, alloys, ceramics, composites, etc. These subjects cover fundamental and applied research and engineering aspects.

We want to foster lively discussions and future international collaborations on this important and stimulating field with this conference.

We choose the venue of the conference as the exciting city of Rostock with all the amenities of such a place in a very nice surrounding and with the possibility to explore the old and new city and even excursions to historically interesting tourist sites like Old City, Warnemünde etc.

We wish you a very pleasant, joyful, interesting and stimulating conference at the Rostock University, GERMANY.

THE ORGANIZING COMMITTEE

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Keynote Presentations

THERMOPHYSICAL PROPERTIES OF MODERN FUELS

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Egon HASSEL is Professor and chair of Technical Thermodynamics at the University of Rostock in Germany since 1999. He studied physics at Technical University of Aachen, Germany, and went early into Mechanical Engineering, where he received his PhD at Technical University of Aachen and later his Habilitation at Mechanical Engineering from Technical University of Darmstadt, Germany. His interests mainly cover the fields of energy technique, IC engine combustion and measurements of thermodynamic properties. In November 2012 he received an honorary doctorate from Azerbaijan Technical University in Baku.

Internal combustion engines driven with diesel fuel are attractive in comparison to gasoline driven engines, because of relative low CO_2 emissions, high power and reliable functionality. Engineering and environmental challenges concerning diesel engines are the amount of emissions from the engines as acoustic noise, and gases like nitrogen oxides (NO_X), carbon monoxide (CO), unburned hydrocarbons (HC), soot and nano-particles, and of course carbon-dioxide (CO_2) emissions, the latter contributing to the climate warming experienced worldwide.

The stringent emission standards set by the governments require advanced diesel engines technology with improvement of the primary injection and combustion processes within the engine combustion chamber. One important development successfully applied to meet the legal requirements for emissions of diesel engines is the use of a common rail for fuel injection into the primary combustion chamber. This type of fuel injection uses a single fuel pump to feed fuel to a manifold, aka common rail, from which the fuel is fed to the fuel injectors for each cylinder in the diesel engine.

Another current development is the use of alternative fuels instead of fossil diesel or mixtures of alternative fuels and fossil diesel, so-called blends. In general, in dependence on the fuel properties the injection rate and the combustion process with alternative fuel in diesel engines, engine parameters have to be properly adjusted, sometimes engines can run without modification. Alcohols have been proposed as an alternative to conventional fossil gasoline or diesel fuels and usage of these strongly increased during the last years. Thus it is important to have reliable knowledge of the thermophysical properties of the fuel under high pressures, such as density, vapor pressure, viscosity, speed of sound, heat capacity etc. which allows modeling, understanding, and optimizing the injection processes in an internal combustion engine.

Injection rate shaping controlled by the engine management systems is another rather modern development found in many current diesel engines. Current fuel injection systems of compression-diesel engines for transport systems reach pressures up to 200 MPa. It is expected that in near future we will see injection systems with pressures up to 400 MPa in passenger cars. Rate shaping means that the number of injections per cycle and the amount of fuel per injection can be varied and the time duration of one single injection process can be changed. The most important injection parameters, which depend on the physical properties of the fuel, such as distillation range, cloud point, pour point, sulfur content, fuel stability, etc, are the inlet fuel pressure to the injector and the rate of injection which determine the spray penetration and atomization and finally the vaporization.

Upon injection of the fuel in a cylinder, large depressurization of the fuel results in a significant change of the thermophysical properties of the fluid.

For optimal design of diesel engine combustion and high pressure fuel injection process with fuel mixtures concerning understanding, modeling and optimizing spray formation, vaporization, combustion and pollutant formation an accurate knowledge of basic fuel thermophysical properties, like density, vapor pressure, viscosity, speed of sound, surface tension, heat capacity, bulk modulus, etc. as a function of pressure, temperature and composition, is required.

This work presents an application of that method to various ethanol + diesel or 1-butanol + diesel binary fuel blends. The (p,ρ,T) properties at T = (263.15 to 468.15) K and pressures up to p = 200 MPa, vapor pressure at T = (274.15 to 468.15) K, heat capacity at T = (253.15 to 468.15) K at ambient and saturated pressures of these blends, also pure diesel, ethanol and 1-butanol were measured experimentally. An equation of state for fitting of the (p,ρ,T) data of investigated systems has been developed as a function of pressure, temperature and concentration. Various thermophysical properties of these fuel blends, such as isothermal compressibility, isobaric thermal expansibility, thermal pressure coefficient, internal pressure, specific heat capacities at constant pressure and volume, speed of sound, isothermal exponent were calculated at high pressures up to 200 MPa and temperatures, for which the (p,ρ,T) properties were studied experimentally. The excess molar volumes V_m^E of ethanol or 1-butanol and diesel binary mixtures at T = (263.15 to 468.15) K, pressures up to p = 200 MPa were calculated using the experimental (p,ρ,T) data values of fuel blends, pure diesel, ethanol and 1-butanol.

THERMOPHYSICAL PROPERTIES OF POLYMER NANOCOMPOSITES REINFORCED WITH CARBON BASED MATERIALS

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Polymer nanocomposites have found extensive applications in automotive, electronics, aerospace, batteries, energy technology etc. The thermal management is significant for the lifetime, reliability and performance of electronic devices. With integration, functionalization and miniaturization of electronic devices, the thermal dissipation became a critical problem. Polymer nanocomposites with improved thermal properties are in high demand to solve this problem. Carbon based materials, such as carbon nanotubes (CNTs), graphene (GNP), graphite, carbon etc., are the most attractive among reinforcements for polymer nanocomposites due to their low density, high electrical, mechanical and thermal properties. As is known, small amounts of carbon based filler materials can considerably enhance the thermophysical properties of polymer nanocomposites. Although of their high prices, CNTs and GNP are the most attractive fillers due to their very high thermal and electrical conductivities compared to other carbon based materials. Many studies in recent years have been conducted on thermal conductivity of polymer nanocomposites reinforced with CNTs or GNP in the literature. Zakaria et al [1] investigated the effect of the MWCNTs and GNP on the thermal properties of epoxy nanocomposites at various weight fraction of filler concentration. It is found that the epoxy reinforced with GNP showed higher enhancement in thermal properties compared to epoxy/MWCNTs nanocomposites. The reason is that GNP has better structural quality than MWCNTs, based on Raman and XRD analysis. He et al [2] found that thermal conductivity of polymer-bonded composites can be enhanced by carbon based materials, especially CNTs/GNP materials. The thermal conductivity results of high density polyethylene (HDPE)/MWCNTs nanocomposites obtained by Evgin et al [3] were compared with the results of Chirtoc et al [4] on HDPE/expanded graphite (EG) nanocomposites, show that EG fillers give better thermal conductivity enhancement than MWCNTs due to lower interface resistance, more rigid structure and higher surface area of EG as compared to MWCNTs fillers. Other experimental results of recent publications were compared with other types of conductive fillers such as metallic and ceramic fillers, showing that carbon based fillers give better enhancement. This subject is still open to investigation due to some controversial results in the literature.

Keywords: polymer, carbon based materials, nanocomposites, thermal properties

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ADVANCED THERMODYNAMICS: A JOURNEY OF MY EXPERIENCE IN WRITING A TEXTBOOK ON THERMODYNAMICS & JOULE-THOMSON INVERSION CURVES: A MEASURE FOR QUALITY OF EQUATIONS OF STATE

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Advanced thermodynamics is becoming a subject of renewed interest for its practical applications to related topics. The requirement to solve complex engineering systems along with the availability of computer power and software resources has rendered this interest more complex. Therefore, new textbooks with modern tools are in demand.

The first part of this presentation will be about the author’s experience in writing a textbook on advanced thermodynamics in addition to previous experiences on writing books for modelling. The second part of this presentation will be about a validation technique applied to some of the well-known EOSs, including van der Waals, Dieterici, and Redlich-Kwong models. Equations of State (EOS) are mathematical models that have a lot of practical applications to solve thermodynamic engineering problems. The validity of any proposed EOS is required in order to have a reliable model for material behaviour prediction under different thermodynamic conditions. The results of this validation study and mathematics will also be presented.

GAS THERMAL CONDUCTIVITY MEASUREMENTS FOR APPLICATIONS RELEVANT TO LNG PRODUCTION

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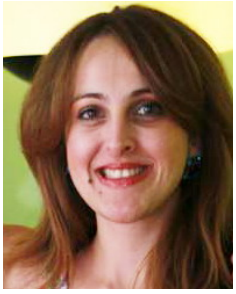

The thermal conductivity of hydrocarbon mixtures is important to the design of heat transfer equipment used in gas gathering, processing and liquefied natural gas (LNG) production facilities. These facilities operate at high pressures and over a wide range of temperatures. Without accurate knowledge of the fluid's thermal conductivity at the relevant conditions, engineers tend to over-design equipment resulting in higher capital and operating costs. In this work, thermal conductivity measurements of a binary (0.9 CH_4 + 0.1 C_3H_8) gas mixture are presented. The thermal conductivity measurements were performed at temperatures from (200 to 423) K and at pressures up to 31 MPa using the transient hot-wire technique. This is a high accuracy technique where the fluid's thermal conductivity is calculated from the transient temperature rise of a resistively heated wires. The thermal conductivity measurements employed used a new custom transient hot-wire sensor consisting of two parallel 10 μm-diameter platinum wires, placed on different arms of a Wheatstone bridge. The operation of the new sensor was validated by conducting gas thermal conductivity measurements of methane, propane and argon in the same temperature and pressure range.

The new experimental thermal conductivities obtained in the current work were compared with published data and results calculated using models implemented in REFPROP 9.1. For pure fluids this software package uses reference equations of state to calculate the density and reference correlations to calculate the thermal conductivity. For mixtures the GERG 2008 equation of state is used to calculate the density and the extended corresponding states (ECS) correlation is used to calculate the thermal conductivity. The percentage deviations of the pure methane, propane and argon data from thermal conductivities calculated using the reference equations using in REFPROP 9.1 were within ± 2 %, which is within the uncertainty of the current measurements. For the binary (0.9 CH_4 + 0.1 C_3H_8) mixture the relative deviations of our measurements from those calculated using ECS model were within ± 4 %. Currently, preparations for measurements of ternary CH_4 + C_3H_8 + C_7H_{16} mixtures with same apparatus are underway for similar ranges of temperature and pressure.

Oral Presentations

OXIDATION OF NAPHTHENE-PARAFFIN HYDROCARBONS IN THE PRESENCE OF Fe-Mn MODIFIED FULLERENES

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The scientific and practical interest of researchers directed towards finding effective solutions for improving the properties of the catalysts. One such modification is the object materials various additives, which will greatly improve the characteristics of the materials. To this end, C60 / C70 has been modified metal by chemical vapor deposition (chemical vapour deposition, CVD) [1]. For the modification of fullerene was used ferrocene and manganese naphthenate. Further, the thermal analysis was conducted of the obtained sample by TG / DTG (Fig. 1.), thereby defining when modified fullerene metals increases its stability. Therefore, the object can be used in oxidation reactions of hydrocarbon oil as the catalyst system.

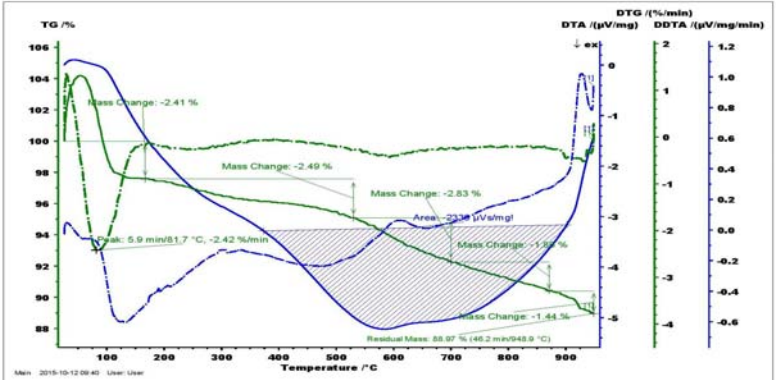

Figure 1: TG/DTG of Fe-Mn/C_{60}/C_{70}

Table 1. Oxidation of petroleum hydrocarbons in the presence of a catalyst novel synthesized Fe-Mn / C_{60} / C_{70}, at a temperature of - 135-140° C. (amount of arom.hydrocarbons in mix - 1.0%).

Named of catalyst	Amount of catalyst, %	Amount of metals in catalyst %	Time of reaction, hour	Acidity number, mgKOH/g	Yield of acids OSOA+SOA,%
C_{60}/C_{70} [2]	0.01	0	6.0	45.3	16.0
Fe-Mn/ C_{60}/C_{70}	0.09	3.24 3.24	5.0	40.0	47.0
Fe-Mn/ C_{60}/C_{70}	0.06	3.24 3.24	5.0	43.1	47.0
Fe-Mn /C_{60}/C_{70}	0.06	4.46 1.62	5.0	67.2	33.8

OSOA-oxy synthesis oil acids, SOA - synthesis oil acids.

As seen from the table of results, which used catalyst actively promotes the conversion of oxygen containing products and total yield of acid is increased to 47%. The metal content of fullerene in equal amounts gives best results than with different amounts.

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OBTAINING OF MONOALKYL (C_8-C_{12}) PHENOLFORMALDEHYDE OLIGOMERS FUNCTIONALIZED BY IMIDAZOLINES AND AMIDOAMINES

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Control of the corrosion of metals [1] is an important area of technical, economic, environmental activities. The modification of phenol-formaldehyde oligomers with nitrogen-containing compounds in order to obtain materials with a complex of required properties for the protection of metals from corrosion is of great interest. Since, modification of nitrogen-containing compounds reduces the content of free phenol, providing ecological safety and stability of the product, contributes to the enrichment of the latter with polar fragments, the presence of which determines the protective effect both as anticorrosion coatings and inhibitors. Previous studies [2,3] have yielded positive results on the use of nitrogen-containing phenol-formaldehyde oligomers (PhFO) for the production of protective coatings and conservation liquids. However, the limited solubility of the rich in polar PhFO fragments in hydrocarbon solvents, oils and other nonpolar media narrows the field of their application. In this connection, there is a need to observe the balance of polar and nonpolar groups, which satisfies both solubility and protective properties. To achieve good solubility in oils, modified with nitrogen-containing compounds oligomers based on monosubstituted alkylphenols with C_8-C_{12} alkyl groups in the p-position and formaldehyde were synthesized. Imidazolines and amidoamines are synthesized on the basis of distilled natural petroleum acids (DNPA) and polyamines - diethylenetriamine (DETA), triethylenetetraamine (TETA), polyethylenepolyamines (PEPA). Synthesis of imidazolineswas carried out according to a known procedure [4] by the interaction of DNPA with DETA, TETA, and PEPA in various molar ratios, at the temperature of 240 °C and a reaction time of 3-3.5 hours. Synthesis of amidoamineswas carried out analogously to the preparation of imidazolines, but at the temperature of 140 °C in various molar ratios of acids to polyamines. When choosing molar ratios, special attention was paid to the presence of amine fragments with mobile hydrogen atoms in the imidazolines. Synthesized imidazolines and amidoamines are viscous resinous products of dark brown color. Synthesis of monoalkyl (C_8-C_{12}) PhFO modified by imidazolines and amidoamines was carried out by the reaction of phenol with formaldehyde in an acidic medium at the temperature of 98-100 ° C until the appearance of a turbidity indicating the formation of condensation centers and the formation of an oligomeric chain, followed by the addition of imidazolines or amidoamines by parts at low temperature (~ 50 ° C) and an increase in temperature to 98-100 °C, at which the process takes another 1 hour. The final products are a resinous mass of light or dark brown, and also brown. The synthesized oligomers were studied by IR spectroscopy. Based on the results of the analysis, a probable mechanism and the proposed structure of the modified oligomer are proposed.

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SOLAR LIGHT PHOTODETECTORS BASED ON NANOCRYSTALLINE ZINC OXIDE CADMIUM DOPED/P-SI HETEROJUNCTIONS

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Zinc oxide semiconductor is a promising material for various optoelectronic applications such as visible light and UV detectors. The transparent undoped and Cd doped ZnO thin films were grown on p-type Si substrates to fabricate undoped and Cd-ZnO/p-Si heterojunctiondiodes. X-ray diffraction patterns confirmed the polycrystalline nature of the films. A combination of cubic CdO and hexagonal wurtzite ZnO phases was observed. The transmittance measurements indicate that the films have transmittance between 83% and 94% for visible and near infrared wavelengths and a direct band gap 3.27 to 3.19 eV range dependent on Cd content.

The photoresponse properties of the diodes under various illuminations were investigated. The diodes exhibit a low open circuit voltage and high photo current values. Capacitance voltage (C-V) measurements suggest the presence of continuous distribution of interface states over the frequency characterization range. The diode having 0.1% Cd doped Zno showed the best photosensitivity of applied reverse bias, with the photoresponsitivity of 3.6 x 10^{-4}. The obtained results indicate that the Al/p-Si/Cd-ZnO/Al diode can be used as photodetector in optoelectronic applications.

KEYWORDS: Zincoxide, cadmium doped Photodiode, Photoresponse properties, sol-gel, optical properties.

NOVEL APPROACHES FOR VISCOMETRIC PREDICTION OF BINARY AND HIGHER ORDER LIQUID MIXTURES

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As a transport property of critical importance, viscosity of liquid mixtures, especially beyond the binary has been a subject of active interestasthey serve as a very vital and versatile tool for flow measurements and to study intermolecular interactions in liquid mixtures particularly in the field of petrochemical and reservoir engineering. The need for development of newer models for theoretical evaluation of viscosity is a matter of considerable significance and various theories have been proposed by several workers over the years. Keeping this in mind, we have tried to modify some of the existing predictive equations and proposed two new equations for predicting the absolute viscosity of binary, ternary and higher order liquid mixtures at varying temperatures.The results indicate that all the proposed models are capable of predicting viscosity better than most of the well established relations exhibiting remarkable predictive capability. The obtained results have been compared with few predictive and correlative approaches in literature by taking absolute average percentage deviation (AAPD) as the criterion. The improvements in AAPD values are seen to be as high as 80.86 times (8085.7%) for binary and 5.85 times (585 %) in case of ternary system in some cases.

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COMPUTER PROGRAMS AND DATABASES FOR THERMODYNAMIC MODELING OF COMPLEX CHEMICAL EQUILIBRIUM

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Thermodynamic modeling is widely used now for theoretical investigation of equilibrium composition and properties of complex chemically reacting systems. Theoretical foundations for such a modeling were laid by J. Gibbs in XIX century, but only accumulation of thermochemical data, development and wide spread of computers make it possible to use the Gibbs approach for solving the practical problems. First computer-oriented algorithms for the calculation of complex chemical equilibrium were developed in 1940-1950 years, but the problem of chemical equilibrium calculation is so complicated that new algorithms and programs for its solution still appear. One of the problems of chemical equilibrium calculation is the complexity of thermodynamic model. Even the simple thermodynamic model of methane in air combustion may require information on thermodynamic properties of more than 200 substances – potential combustion products. That is why a database on thermodynamic properties of pure substances is a necessary part of thermodynamic modeling software package.

In our presentation we briefly describe some popular in Russian Federation computer programs and databases for the thermodynamic modeling of complex chemical equilibrium. Among them are TERRA, developed by Boris Trusov, professor of Bauman Moscow Technical State University, IVTANTHERMO for Windows developed in Glushko Thermocenter of Russian Academy of Sciences.

There are two kinds of software packages for thermodynamic modeling, namely specialized programs and relatively universal programs. The difference is often rather subtle. Specialized programs as one can expect often are designed to solve only one class of problems and do it well. General purpose programs use only simple models such as ideal gas equation of state and ideal solution model, but they can be applied in many branches of science and industry. Both TERRA and IVATANTHERMO for Windows are general purpose software tools.

Database IVTANTHERMO is the result of a long term project on development of the reference book on thermodynamic properties of individual (pure) substances, similar to NIST-JANAF thermochemical tables.

APPLICATION OF NEW CALORIMETRIC METHODS FOR RESERVOIR FLUIDAL SYSTEMS STUDY

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The presentation analyzes the phase behavior of fluidal gas condensate systems in low-temperature reservoirs of tight reservoir rocks. A number of deposits of the new gas-condensate and oil-gas-condensate fields of Siberia is characterized by these conditions. As examples are Chayandinskoe oil-gas-condensate field, Kovyktinskoye gas-condensate field and Bovanenkovskoye oil-gas-condensate field. A method of precision adiabatic calorimetry for investigation of phase behavior of fluidal gas condensate systems was applied. The thermodynamic properties, phase behavior and kinetics of phase transitions of liquid and gaseous hydrocarbons have been studied in the temperature range from 100 to 370 K and in pressure range from 0.1 to 40 MPa. A method of precision adiabatic calorimetry makes possible to construct the phase diagrams of hydrocarbon mixtures, as well to determine with higher accuracy PVT data of condensate dew points. Phase transitions are determined by the discontinuity of measured specific heat and temperature derivative of pressure at constant volume. The method makes possible to study the phase diagrams of reservoir fluids, including diagrams with a low condensate ratio, as well to determine PVT data of condensate dew point with higher accuracy. Particular attention is paid to the hydrocarbon mixtures with low content of high molecular components (content of C_{5+} components is less then 2.0 mol%) due to the fact that standard methods with the use of conventional PVT experiments not guarantee the efficiency and accuracy of phase diagram. Our investigations showed that phase behavior of hydrocarbon mixtures with low content of high molecular components is qualitatively differed from traditional phase behavior. The region of phase state of hydrocarbon mixtures with low content of high molecular components includes the extensive domain of uncertainty and cannot be studied by conventional PVT experiments and cannot be prognosticate theoretically. Besides, the results of experiments showed that phase behavior of hydrocarbon fluid in porous medium is transformed drastically by the porous medium effects (sorption/desorption processes). Capillary effects (capillary evaporation and capillary condensation) and their influence on phase behavior of hydrocarbon fluids were studied. Also a method of adiabatic calorimetry allows to determine with higher accuracy PVT data of hydrate formation and compositions of vapor-liquid and sorbed phases in reservoir. Hydrate formation of pure liquid and gaseous hydrocarbons and their mixtures in water saturated porous media were studied. Obtained data are topical for the new gas-condensate and oil-gas-condensate fields of the Republic of Sakha (Yakutia), characterized by abnormally low reservoir temperatures.

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TECHNO-ECONOMIC ANALYSIS OF A PHOTOVOLTAIC POWER PLANT

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Energy is an essential factor for development and economic growth of the countries. According to main scenario of International Energy Agency [1], it is expected that global energy demand will grow 30% till to 2040. Today, fossil fuels, such as oil, coal and natural gas etc., supply approximately 86% of global primary energy [2]. Paris Climate Agreement [3] suggested shifting the resources away from polluting fossil fuels to clean energy and therefore, renewable energy has gained more important role since it is clean, safe and sustainable.

Today, renewable energy sources, including hydro, constitute nearly 34 percent of total energy generating capacity in Turkey. Although Turkey has a significant potential for solar energy, installed photovoltaic (PV) power capacity has reached only just 832 MWe by the end of December 2016 and it is less than 1% of overall electricity production. It is aimed to increase this capacity up to 5000 MW by 2023 [4]. Therefore, much more attention should be paid for the techno-economic analyses of PV power plants.

This study presents a technical and economic evaluation of a PV plant with installed capacity of 0.883 MWe. The selected location is in the town of Dursunbey in Balıkesir (39°35'16" N, 28°37'39" E), in the South Marmara Region of Turkey. Three PV panel mounting designs, fixed-tilt, single-axis solar tracking and dual-axis solar tracking, are considered for comparisons of turnkey costs, internal rate of return values, levelized costs of electricity (LCOE), net present values and payback periods of the systems. The calculations were made using the PVSyst software and Meteonorm data. The results are presented in the following table.

	Fixed-tilt, 30˚	Single-axis solar tracking	Dual-axis solar tracking
Turnkey cost (USD)	1,160,000	1,313,500	1,520,000
Internal rate of return (%)	12.01	12.96	12.34
LCOE (USDcent / kWh)	5,340	5,484	6,033
Net present value (USD)	1,638,732	2,029,778	2,162,884
Payback period (years)	7.2	6.8	7.2

The results show that the fixed-tilt and dual-axis designs have the payback periods of 7.2 years, whereas the payback period is 6.8 years for the single-axis system.

KEYWORDS: solar energy, photovoltaics, techno-economic analysis, levelized cost of electricity.

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DETERMINING THE OPTIMUM REFRIGERANT FOR STANDARD REFRIGERATION CYCLE BY USING GENERALIZED LEE_KESLER EQUATION OF STATE

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Selection of correct refrigerant to obtain maximum possible COP in a refrigeration cycle is quite important. Cubic equation of states such as Soawe and Peng-Robinson and Lee-Kesler EOS can be written in general form as a function of Pitzer acentric factor. Pitzer acentric factor is defined for reduced temperature $T_r=T/T_c$ =0.7 as a function of reduced vapor pressure $P_{vpr}(T_r)$ by the following formula: $\omega = -\log [P_{vpr}(T_r=0.7)]-1.0$. Out of this equation of states Lee-Kesler EOS is a converted form of Benedict-Webb-Rubin (BWR) EOS and gives more accurate results compare to the cubic equation of states. Generalized compressibility factor, generalized enthalpy and entropy charts are obtained by using Lee-Kesler EOS. In this study standart gas cycle is modelled by using Lee-Kesler equation of state and cycle is optimized by using stochastic optimisation methods for the to Pitzer acentric factor to give the maximum possible COP values for the given conditions. Optimal Pitzer acentric factor is compared with the acentric factor of the actual gases and the closest candidates are selected to be utilised in actual refrigeration cycle.

KEYWORDS: Thermodynamics, Lee-Kesler equation of state, standard refrigeration cycle, stochastic optimisation

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MODELLING OF R290 (PROPANE) EQUATION OF STATE

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When simulating refrigeration systems or equipment, knowledge of refrigerant thermodynamic properties is required. Properties of refrigerants are a major part of international trade, therefore, it is a subject of interest of international standards. Natural refrigerants, such as propane (R290) are getting more interests in recent years due to low greenhouse effect. In this study a computer model was developed based on National Institutes of Standards and Technology of United States (NIST) equation of state and cubic spline curve fitting models developed by using saturation thermophysical properties of the refrigerants and refrigerant mixtures. Java programming language was used to model equation of state. The thermodynamic properties of R290 were compared with REFPROP 9.0. It shows that the total mean deviations of the new model are less than 0.5%. Equation of state is applied to develop standard refrigeration cycle for R290, furthermore a bath optimisation algorithm is developed to optimize cycle properties for the bast COP values.

KEYWORDS: Thermodynamics, R290 equation of state, thermodynamic properties, standard refrigeration cycle

VISCOSITY AND THERMAL CONDUCTIVITY OF MAGNETIC NANOFLUIDS

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Magnetic nanofluids are colloidal mixtures which consist of magnetic nano-sized particles suspended in a base fluid such as water, oil, ethylene glycol etc. The typical magnetic nano-sized particles could be maghemite (γ–Fe_2O_3), magnetite (Fe_3O_4) or cobalt ferrite ($CoFe_2O_4$) etc. Magnetic nanofluids have many potential application such as sealing, lubricating, ink jet printers, electronics cooling, clutches, dampers, heat transfer applications, biosensors, drug delivery, medicine [1]. Requirement to miniaturized devices in different areas has increased in recent years due to the technological developments. Consequently, microelectromechanical systems (MEMS) which are micro-sized systems have begun to be used in heat transfer, biomedical, electronic and space applications. The ability of being manipulated by an external magnetic field of magnetic nanofluids made them considerable for microfluidic systems which are the one of the most common among MEMS. Because of the implementation potential in microfluidic systems of magnetic nanofluids, the thermophysical properties of them need to be investigated before employing them inside any system. One of the pioneering study on the viscosity of magnetic nanofluids by McTague [2] indicated that the viscosity of magnetic nanofluids changes when they are exposed an external magnetic field both parallel and perpendicular to the flow. Since then, several studies have been conducted on thermophysical properties of magnetic nanofluids under external magnetic field. In this study, papers focused on the viscosity and thermal conductivity of magnetic nanofluids with or without external magnetic field have been reviewed in terms of particle size, vol. or wt. concentration, temperature and magnetic field magnitude and direction. The results revealed that the relative viscosity and the relative thermal conductivity of magnetic nanofluids could increase up to 256 % and 300 %, respectively, in the presence of external magnetic field.

Keywords: magnetic nanofluid, magnetic field, viscosity, thermal conductivity, microfluidic systems, MEMS.

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THERMODYNAMIC PROPERTIES OF SOME HETEROCYCLIC BIOLOGICALLY ACTIVE COMPOUNDS

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Heterocyclic compounds with furan cycle are used as starting compounds during synthesis of biologically active substances with antioxidant, antifungal, antitumor and antibacterial properties. The investigated nitro-containing isomeric compounds are: 5-(2-nitrophenyl)-furyl-2 oxime (I), 5-(3-nitrophenyl)-furyl-2 oxime (II), 5-(4-nitrophenyl)-furyl-2 oxime (III), β-(5-(2-nitrophenyl)-furyl-2-prop-2-enoic acid (IV), β-(5-(3-nitrophenyl)-furyl-2-prop-2-enoic acid (V), β-(5-(4-nitrophenyl)-furyl-2-prop-2-enoic acid (VI), ethyl esther of ά-cyano-β-[5-(2-nitrophenyl)-furyl-2]-prop-2-enoic acid (VII), ethyl esther of ά-cyano-β-[5-(3-nitrophenyl)-furyl-2]-prop-2-enoic acid (VIII), ethyl esther of ά-cyano-β-[5-(4-nitrophenyl)-furyl-2]-prop-2-enoic acid (IX), ά-cyano-β-[5-(2-nitrophenyl)-furyl-2]-prop-2-enoic acid amide (X), ά-cyano-β-[5-(3-nitrophenyl)-furyl-2]-prop-2-enoic acid amide (XI), ά-cyano-β-[5-(4-nitrophenyl)-furyl-2]-prop-2-enoic acid amide (XII).

Investigated compounds are in solid state under normal conditions. The substances were identified by ^{1}H NMR spectra data using Varian-600 (600 MHz) device. Purity of the compounds was confirmed by the results of chromatography using Agilent 1100 HPLC with diode matrix and mass-selective detector on Zorbax SB-C18 column, 4.6mm×15mm, eluent A – acetonitrile-water with 0.1% TFA (95:5), no impurities were found. Sublimation enthalpies ($\Delta_{sub}H_{Tm}$) were calculated from the temperature dependances of saturated vapor pressures, determined by Knudsen’s integral effusion method. Sublimation enthalpies for substances (X–XII) were determined from differential-thermal and thermo-gravimetric analysis data, as sum of vaporization and fusion enthalpies at 298K calculated using equations from [1]. Adjustment of $\Delta_{sub}H_{Tm}$ to 298K was conducted using equations in [1, 2]. Combustion and formation ($\Delta_f H_{298}$, s) enthalpies in crystalline state were determined using bomb combustion calorymetry on V-08-MA with isothermal shell. Formation enthalpies in gaseous state ($\Delta_f H_{298}$, g) were calculated using average values of sublimation enthalpies at 298K. Results of thermodynamic studies are shown in the Table 1.

Table 1. Thermodynamic properties of the investigated compounds

Compound	T_m, K	$\Delta_{sub}H_{Tm}$,	$\Delta_{sub}H_{298}$, [1]	$\Delta_{sub}H_{298}$, [2]	$\Delta_f H_{298}$, (s)	$\Delta_f H_{298}$, (g)
		kJ/mol				
I	387.3	111.8±3.8	115.4±4.3	117.2±4.3	-14.6±2.4	101.7±6.5
II	404.9	109.0±3.3	113.3±3.7	115.5±3.7	-50.1±2.5	64.3±5.8
III	421.8	113.6±4.0	118.5±4.5	121.1±4.5	-58.0±2.6	61.8±6.9
IV	430.4	208.6±3.6	214.7±4.0	217.6±4.1	-408.6±3.3	-192.4±6.6
V	446.6	193.4±4.2	200.2±4.8	203.5±4.7	-428.1±3.6	-226.3±7.6
VI	450.8	194.6±3.9	201.6±4.5	204.9±4.4	-431.3±3.4	-228.0±7.1
VII	412.3	139.3±3.1	145.9±3.6	148.6±3.5	-247.8 ± 2.4	-100.6±5.6
VIII	439.3	142.7±3.5	150.8±4.0	154.2±3.9	-277.4 ± 2.2	-124.9±6.0
IX	441.4	176.0±4.8	184.2±5.3	187.7±5.4	-306.0 ± 4.4	-120.1±8.7
X	-	-	173.0±5.8	-	-81.7 ± 4.8	91.3±7.5
XI	-	-	233.5±6.0	-	-106.9 ± 3.7	126.6±7.0
XII	-	-	251.2±7.3	-	-129.9 ± 2.9	121.2±7.8

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AN INVESTIGATION ON THE VISCOSITY AND THERMAL CONDUCTIVITY OF POLYVINYLPYRROLIDONE / DE-IONIZED WATER SOLUTION

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The nanofluids are considered as the next generation heat transfer fluid because of their superior thermophysical properties. The unstable nature of nanofluids constitutes a major challenge to their use in many potential application areas [1, 2]. Due to the high surface energy of the nanoparticles, the nanofluids have tendency to aggregate which causes instabilities and quick settling down of the particles [3]. In order to reduce the aggregation and enhance the dispersion of nanoparticles, surfactants are added into nanofluids.

Polyvinylpyrrolidone (PVP) is one of the surfactants commonly used in the preparation of nanofluids. PVP prevents the aggregation of nanoparticle and controls the average particle size and shape by providing a steric barrier on particle surface [4]. Since the PVP influences the thermophysical properties of the nanofluids, the comments on the heat transfer properties of the nanofluid should also include the effect of PVP [3]. However in the literature, most of the studies that use surfactant, neglect to evaluate the effect of it on thermophysical properties of nanofluids. Moreover, there are limited studies on the thermophysical properties of PVP-liquid mixtures. So, the aim of this study is to investigate the effect of adding PVP on thermophysical properties of water. For this reason, viscosity and thermal conductivity of PVP-DIW solution were investigated as a function of temperature and molecular weight. The viscosity and thermal conductivity were measured by SV-10 viscometer and 3ω method, respectively. Viscosity of the samples decreases by increasing temperature while it increases by increasing molecular weight of PVP. Moreover, typical Newtonian behavior was observed for the samples by using Brookfield viscometer, at 25 °C. The temperature and molecular weight have no significant effect on the thermal conductivity. Also, the results were compared with the literature data.

KEYWORDS: Surfactant, polyvinylpyrrolidone, nanofluid, thermal conductivity, viscosity

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ANALYSIS DERIVATOGRAFIC AND THERMOPHYSICAL PROPERTIES OF COMPOSITES WITH FILLERS OF BIOLOGICAL ORIGIN

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The work is devoted to obtaining differential thermal gravimetric analysis and determination of physico - chemical parameters of composite materials in the matrix of low density polyethylene with fillers of biological origin - fish bone (FB) and aluminum nanoparticles. To produce filler - fish bones are cleaned and rinsed thoroughly with clean water, heated to a temperature of 50^0C, kept at this temperature for 10 minutes to an hour depending on the size of the bones. After that bones are crushed to a size of 100 microns. Volumetric content of the filler biological origin in the studied composites ranged from 3 to 7%, and volume content of Al_2O_3 nanoparticles was 1%. Composites were obtained from a homogeneous mixture of filler powder and LDPE using a hand press heated at a temperature of 120^0C and a pressure of 15 MPa. the crystallization mode - quenching-cooling of the sample in an ice-water mixture. The thus obtained film samples were approximately 200 microns thick. Differential Thermal Analysis (DTA) were carried out on derivatograph "Perkin Elmer" STA 6000 and NETSCHE DSC 204 F1 Phoenix. The samples were heated in the temperature range 60-180^0C in a platinum crucible rate of 10 K / min. The heats of melting composites were determined by the melting area of the original crystalline phase LDPE. The degree of crystallinity (K) was determined by the method of dividing the heat of fusion of studied composites at a heat of fusion LDPE, assuming the heat of fusion LDPE is ΔH = 286.7 kJ / kg. [1].

The entropy change and the Gibbs energy were determined from experimental data of the specific heat and entalpiya composites by the method described in [2.].

Table. Thermal and physical parameters of composites LDPE + xvol.%FB and LDPE + xvol.%FB + 1vol.% Al_2O_3.

Composites	The melting temperature, ^{0}C	Heat quantity, mC	Change of enthalpy, C/kg	Energy of activation, kC / mol	Heat capacity, C/kg^{0}C	Changes in entropy, C/mol^{0}C	Gibbs energy, C/mol^{0}C	The degree of crystallization, %
3 vol.% FB	126.29	2070	174,948	0.1749	2,762	1914.473	-66830	61
5vol.% FB	126.81	585	149,394	0.1494	14,463	6702.197	-700512	52
7 vol.% FB	123.98	453	118,220	0.1182	11,093	5331.138	-542734	41
3vol.% FB +1vol.%Al_2O_3	124.73	945	122,955	0.1230	5,378	2327.943	-167409	42
5 vol.% FB +1vol.%Al_2O_3	125.70	1073	123,958	0.1240	11,231	5785.807	-603318	43
7 vol.% FB +1vol.%Al_2O_3	124.86	569	136,518	0.1365	2,789	1307.244	-26704	47

Analysis of the results shows that the dispersed particles fishbone affect all levels of the organization structure of LDPE and thus lead to the complex nature of the kinetics of change of thermal properties of compounded material.

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FEATURES OF MAGNETIC INTERACTION IN COMPOSITES BASED ON SIDERITE AND POLYMER

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Nowadays, it is very actual to develop the new magnetic materials (in particular, systems containing single-domain magnetic nanoparticles), new magnetic materials are widely used in engineering, as they have a record of the magnetic parameters, or an optimal combination of magnetic and other electrical characteristics. These magnetic materials have provided the solution to many technological challenges and significant contribution to scientific and technical progress in the modern world.

The fact is that at the distances of the order of the size of the atom, or about ten atomic dimensions (about a nanometer) are expected new different magnetic effects , as a result of the fact that the range of the exchange interaction, which leads to magnetic ordering (ferromagnetic or antiferromagnetic), amounts to several interatomic distances. In the last decade, has been made some progress in the development of multilayer magnetic films and artificial magnetic structures, in which new effects arise due to the interaction of the "magnetic electron" with artificially created nanoscale structures. In accordance with the principles developed in these devices are used the combination of magnetism and electronics, therefore we can speak of the birth of a new field of magnetism and technology-a magnetoelectric [1-5]. In this paper we set the goal synthesis and study of magnetic resistance in composites based on polymer (PP) and microparticles annealed siderite (Fe, Mn)CO_3. We have investigated the influence of the size of magnetic particles on the magnetic characteristics of composites based on (30-50%) annealed siderite (AS) and (70- 50%) (PP). It is established the presence of a size effect in the studied composites, namely, with a decrease in the size of magnetic particles the value of the coercive force increases, and the remanent magnetization and saturation of the magnetization decrease. It was found that, regardless of the size of the magnetic particles (with the same percentage of the components), the values of M_r, M_s and H_c increase with decreasing.

EXPERIMENTAL DENSITY MEASUREMENTS OF TWO GRAVIMETRICALLY PREPARED NATURAL GAS-TYPE MIXTURES, ONE BEING HYDROGEN-ENRICHED

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The GERG-2008 equation of state is the approved ISO standard (ISO 20765-2) for the calculation of thermophysical properties of natural gas-type mixtures [1]. Natural gas composition varies considerably due to the diversity of origins. Recently, further diversification was generated by adding hydrogen, biogas, or other non-conventional energy gases. A comparison with experimental (p, ρ, T) data of real mixtures can assess the performance, preferably when using a standard mixture of high accuracy in its composition. Mixtures that are prepared by gravimetry according to ISO 6142 qualify best [2].

In this work, density measurements for two gravimetrically prepared synthetic natural gas mixtures are presented. The first mixture resembles a conventional natural gas of 11 components (BAM-G420 or "11M" according to the PTB specification PTB-A 7.63 [3]). The mixture nominal composition (x / mol-%) of 11M is: oxygen 0.5, nitrogen 4.0, carbon dioxide 1.5, ethane 4.0, propane 1.0, n- and isobutane 0.2 each, isopentane, n-pentane, n-hexane 0.05 each, methane 88.45.

The other mixture is a 13-component hydrogen-enriched natural gas mixture with low calorific value to facilitate support to power-to-gas applications that was proposed by the Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM) of the Bureau International des Poids et Mesures (BIPM) for an interlaboratory key comparison (K 118) [4]: hydrogen 3.0, helium 0.5, nitrogen 12.0, carbon dioxide 4.0, ethane 0.75, propane 0.3, n- and isobutane 0.2 each, neopentane, isopentane, n-pentane, n-hexane 0.05 each, methane 78.85. The relative uncertainty of the 0.05 mol-% compounds amounts to 0.06 % ($k = 2$).

Density measurements were performed at temperatures between 260 K and 350 K and at pressures up to 20 MPa, using a single-sinker densimeter with magnetic suspension coupling [5]. 94 data points were recorded for 11M and 99 for the K-118 mixture, respectively, in an isothermal operational mode at 260, 275, 300, 325, and 350 K. The data were compared with the corresponding densities calculated from two reference equations of state, namely GERG-2008 and AGA8-DC92 [6]. A remarkable good coincidence was found for each combination of gas mixture and applied equation of state. The average absolute deviation from GERG-2008 (AGA8-DC92) is 0.027 % (0.078 %) for 11M and 0.095 % (0.062 %) for K-118, respectively. The corresponding maximum relative deviation from GERG-2008 (AGA8-DC92) amounted to 0.095 % (0.127 %) for 11M and 0.291 % (0.193 %) for K-118.

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NEW FORMULATION FOR THE VISCOSITY OF NORMAL BUTANE

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The exact knowledge of thermophysical properties of fluids with industrial importance is required for a more accurate basic design of compressors, gas turbines, and gas pipelines as well as cooling cycles and chemical processes. In contrast to the thermodynamic properties, the transport properties of normal butane, particularly in the region near to the critical point, are not sufficiently well-known. The current NIST standard database REFPROP 9.1 of Lemmon et al. (2013) recommends the viscosity correlation of Vogel et al. (1999), which is characterized by standard uncertainties of up to 3% in its range of validity applying an outdated equation of state of Younglove and Ely from 1987. Due to the fact that REFPROP 9.1 approves the reference equation of state of Bücker and Wagner (2006) for the thermodynamic properties of normal butane, there is a basic necessity for developing a new viscosity formulation for this working fluid.

Recently, very accurate viscosity measurements were performed by Herrmann and Vogel (2015) using a vibrating-wire viscometer in combination with a single-sinker densimeter. The standard uncertainty of these data was conservatively estimated to be 0.3%. Hence, they are considered to be primary data. In addition, viscosity measurements by Küchenmeister and Vogel (1998), whose results have already been used by Vogel et al. (1999) when generating their correlation, were re-evaluated (2017), so that they are qualified for being primary data, too.

Applying the new reference equation of state of Bücker and Wagner (2006) together with the improved data situation in the dense-gas region, a new viscosity formulation for normal butane was generated using the structure-optimisation method by Setzmann and Wagner (1989). The new formulation concept incorporates four contributions concerning the zero-density viscosity, the initial-density dependence, the near-critical region, and the higher-density terms of the residual viscosity. The first two contributions are completely treated separately using little support of the kinetic theory. The critical-enhancement terms related to the near-critical region were slightly pre-treated with respect to the choice of some parameters. At the end, the bank of terms needed in the optimization procedure comprises only terms for the near-critical region and for the higher-density contribution. The latter terms are composed of a combination of double polynomials in the reduced density and reciprocal reduced temperature, some of them combined with a negative exponential function of the reduced density. The validity range of the new formulation extends from the melting line to temperatures of 650 K and to pressures of 100 MPa. The extrapolation and consistency behaviours of the formulation were investigated. Values calculated for the new viscosity formulation were compared with the primary data, used when developing the formulation, and with values resulting from the earlier viscosity correlations of Vogel et al. (1999) and of Quiñones-Cisneros and Deiters (2006).

THE INVESTIGATION OF NANO CARBON PRODUCED PYROLYSIS LIQUID PRODUCTS IN SUNFLOWER OIL BLEACHING PROCESS

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The main task of the presented research was to investigate bleaching process with nanocarbon obtained from pyrolysis of liquid products and as well as to investigate the possibilities of production and main technological properties of sunflower oil. The adsorption of the trace metals, color pigments (carotenes, chlorophyll) in sunflower oil with different types of nano carbon, activated carbon and commercial bleaching earth material have been examined at different temperatures, contact times and bleaching material dosages.

The results showed that, the adsorption of metals and pigments depend strongly on adsorbents amount and the maximum adsorption was reached after using 0.05% nano carbon. Compared with nano carbon, approximately 1% of activated carbon and 1.3% bleaching earth gives same result. Moreover, the removal of pigments by adsorption process on all adsorbents started 15 minutes; nano carbon showed maximum adsorption in 20 minutes, activated carbon and bleaching earth showed maximum adsorbtion in 30 minutes contact time. Also, it was determined that, color and heavy metals reduction increased with increasing temperature from 20 °C to 100 °C for the commercial bleaching earth and activated carbon, so increasing temperature increased activation of these adsorbents. But contrary to expectations, the highest bleaching was obtained at 20°C temperature for nano carbon. Color, free fatty acids (FFA), peroxide value (PV), heavy metals, anisidine value (AV) and other parameters of bleached oil were determined to see oil quality after bleaching process. The results indicated that nano carbon has great potential in the removal of color, metals and other residues from sunflower oil. Anisidine value and peroxide value remaining stable due to low temperature and short time when nano carbon using in the bleaching process. Furthermore, FFA and polycyclic aromatic hydrocarbons (PAHs) have decreased more using nano carbon compared to bleaching earth and activated carbon.

ANTI-QUORUM SENSING ACTIVITY OF KAEMPFEROL LOADED LECITHIN/CHITOSAN NANOPARTICLES

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Quorum sensing (QS) mechanism plays a vital role in many bacterial species, which is found to be implicated in various factors including bacterial pathogenicity and biofilm formation. Therefore interrupting the QS mechanism may be an attractive strategy to develop novel QS-based anti-bacterial drugs. We investigated the quorum sensing inhibitory activity of kaempferol loaded lecithin/chitosan nanoparticles (KAE-LC NP) to compare pure kaempferol in the case of the time dependent stability. The KAE-LC NPs were prepared by using the electrostatic self-assembly technique and characterized in terms of average size, surface charge, morphology and chemical structures. Moreover, in vitro evaluation of the KAE-LC NP system was determined by the anti-quorum sensing activity against *Chromobacterium violaceum* CV026 in a concentration- and time-dependent manner compare to free KAE. KAE-LC NPs have diameters of 270 ± 10 nm, PDI ≤0.2 and net positive surface charge (+56 ± 4 mV) respectively, and are spherical in shape and uniform. It was observed from FTIR spectrum that encapsulation of kaempferol in the KAE-LC NPs was formed by hydrophobic interactions. The KAE-LC nanoparticles at all tested concentration inhibited the production of violacein pigment in *C. violaceum* CV026. In addition, encapsulated KAE in nanoparticle exhibited a significantly anti-quorum sensing inhibition efficacy (75%) against *C. violaceum* at the end of the 45 day storage period. However, free KAE displayed no inhibitory activity at the end of 15 day storage period. These findings lay a foundation for the utilization of the KAE-LC nanoparticles as QS-based sustainable anti-biofilm agents to manage bacterial communication inhibition.

KEYWORDS: Flavonoids, Encapsulation, Nanoparticles, Anti-Quorum Sensing, Sustainable Nanoagents.

PHASE BEHAVIOR AND THE CHANGE IN DENSITY AND VISCOSITY OF HIGHER HYDROCARBONS AFTER INJECTION WITH SUPERCRITICAL CO_2 AT PRESSURES TO 76 MPa AND TEMPERATURES TO 410 K

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Climate change is a real risk, and new technologies are rapidly evolving for efficient capture and confinement of carbon emissions. One of the proven technologies is the injection of CO_2 in hydrocarbon rock formation for sequestration in geological CO_2 storages, and also for recovery of the heavy residual oil in mature oil fields. To accurately model and simulate how CO_2 mixes with heavy hydrocarbons in oil reservoirs, accurate thermodynamic properties of these mixtures should be available at same reservoir conditions. Simulated results of these processes often deviate from those observed in actual operations, depending on the selected simulator software and selected property package, even in the same simulator. Accordingly, the selection of the proper equation of state (EOS) for estimating stream properties is also critical for reliable simulation. In this work we report measurements on phase behavior, density and isothermal compressibility of binary mixtures of CO_2 + *n*-decane and CO_2 + *n*-pentadecane, at pressures up to 76 MPa and temperatures from (313 to 410) K. We also report data on how viscosity of a heavy hydrocarbon (2, 6, 10, 15, 19, 23-hexamethyltetracosane with a molar mass of 410 g/mol) is dramatically reduced, as supercritical CO_2 is injected in it, using a custom-made capillary viscometer while density is simultaneously determined from direct measurements of the resonant frequency of a vibrating U-tube using a commercial lock-in amplifier. Our results are compared with all previous experimental data in literature, and with predictions from different EOS: cubic PR; virial BWRS; perturbed-chain statistical associating fluid theory PC-SAFT; and multi-parameters GERG-2008, and with viscosity models commonly used in chemical and petroleum simulators such as Lorenz-Bray-Clark and Pedersen-Wu. The accuracy of experimental data and challenges with the experimental technique are also discussed.

IDENTIFYING NEW SORPTION SYSTEMS FOR THERMAL ENERGY STORAGE BASED ON THERMOPHYSICAL PROPERTIES

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Thermal energy storage based on adsorption processes shows huge potential, especially for storing heats at a temperature level of about 500 K. Conventional systems, based on water and often zeolite 13X, become comparatively inefficient below this temperature, since regeneration (i.e. desorption) is not working properly anymore. New sorptive systems based on other adsorbates as well as other adsorbents show huge potential in this respect [Ref]. Thus, the temperature range of about 400 K can be covered better with thermochemical storage systems than in the past.

The major influencing factor for efficiency and effective energy density is the adsorption behaviour. The determination of this non-isothermal behaviour is crucial for the identification of suitable, new storage systems. Promising sorption systems are characterized by a fast decrease of loading upon increase in temperature within the relevant temperature range. Polynomial and other empirical fits of these changes in loading prove to be insufficient for describing the systems in a way appropriate for accessing their efficiency as thermal energy storage. The potential theory by Polányi can be used for this task, but needs to be modified to be applied to all systems.

In this contribution the suitability of different models for describing non-isothermal adsorption behaviour is evaluated and demonstrated. It is outline that some approaches that are seen as superior in parts of the literature are indeed less accurate under closer examination than seemingly weaker alternatives. Furthermore, modifications of existing models are discussed that allow improving the description without introducing parameters that are not based on the respective physics.

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MELTING, CRYSTALLIZATION, AND ROTATIONAL PHASES TRANSITIONS OF PARAFFIN WATER EMULSIONS VIA STATIC AND DYNAMIC LIGHT SCATTERING

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We studied the melting, crystallization, and rotational phase transition behavior of several paraffin ($C_{19}H_{40}$, $C_{20}H_{42}$, $C_{21}H_{44}$, $C_{23}H_{48}$ and $C_{28}H_{58}$) emulsions in distilled water, by means of ultrasonic dispersion, without the use of surfactants. We verify that the emulsions remained stable for more than half year. These samples are emulsions at temperature above the melting point and suspensions below the crystallization temperature. We present the measurements of the paraffin cluster sizes as a function of the temperature, obtained by Dynamic Light Scattering (DLS). In all the prepared emulsion samples the average size distribution obtained is centered around 100 nm both in the liquid and in the solid state of the paraffin. We present the zeta-potential measurements for the emulsions in temperatures well above and below the respective melting/crystallization one. We investigates the behavior of these samples via DLS and via the intensity of scattered light analysis (SLS), both at heating and cooling; we present the determinations for the crystallization and the melting temperature ranges, as well as the rotational phase transitions ones, with good accuracy and reproducibility. They show a good agreement with the literature data. We would like to underline that the melting and crystallization phase transitions are come along with bright imprints on the temperature dependence of the scattered light intensity associated with a change in the refractive index of paraffin. We show that DLS and SLS techniques could be able not only to measure the cluster size in the paraffin emulsions but even to determinate the phase transitions temperatures, task that represents an actual and relevant interest for other scientific communities such as the one involved in the study of the Phase-change material (PCM) products.

SYNTHESIS OF SUPRAMOLECULAR ENSEMBLES ON THE BASIS OF NANO LAYERS OF GRAPHENE OXIDE

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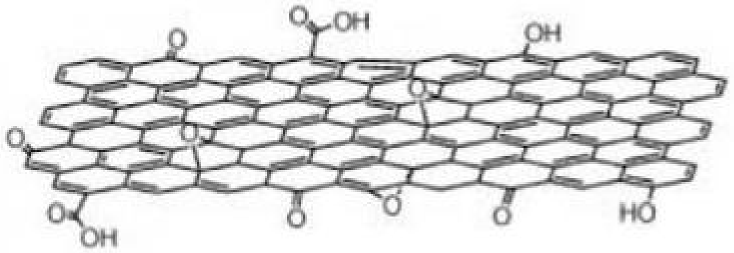
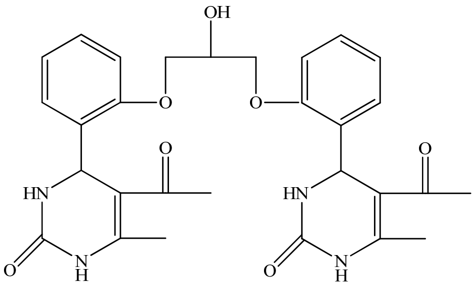
Graphene oxide (GO) is a single-atomic layered material with oxygen-containing groups, made by the powerful oxidation of graphite, which is cheap and abundant. One of the advantages of the GO is its easy dispersability in water and other organic solvents, as well as in different matrixes, due to the presence of the oxygen functionalities.



Functionalization of GO can fundamentally change GO’s properties. The resulting chemically modified graphenes could then potentially become much more adaptable for a lot of applications, for example in optoelectronics, biodevices, as a drug-delivery material and so on.

In this work we report about synthesis of ensembles on the basis of GO nanolayers with silver nanoparticles and PLGA (poly(lactic-co-glycolic acid)). The reason of using of silver is caused by its antibacterial activity, whereas PLGA is a biodegradable and biocompatible copolymer. The following ensembles were obtained: GO-Ag, GO-PLGA, Ag-PLGA and GO-Ag-PLGA. Subsequently, antibacterial activity of obtained ensembles along with individual GO and Ag were investigated against E.coli. It was found that they demonstrate promising antibacterial activities, which allow concluding that they are able to be used in water disinfecting membrane, in fabric to kill bacteria, making clothing odor-resistant or as drug delivery system, which require further investigations.

The next ensembles which was obtained are the ensembles on the basis of GO and dihydropyrimidines I and II. The reason of using dihydropyrimidines is their antiviral, antiproliferative, anti-HIV, anti-malarial, anti-inflammatory, antitumor, antihypertensive activities. Obtained ensembles also demonstrate promising antibacterial activity, which allow concluding that they can be used in water disinfecting membrane or as a drug, which require further investigations.



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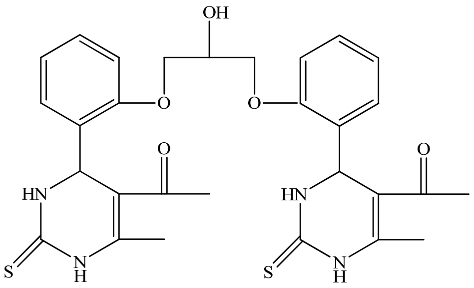

II

SYNTESIS OF ZEOLITE AND GRAPHENE OXIDE SUPPORTED ZERO VALENT IRON, NICKEL, COBALT NANOPARTICLES FOR REMEDIATION PURPOUSES

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Nanoparticles are of great scientific interest as they are, in effect, a bridge between bulk materials and atomic or molecular structures. The interest to nano scale particles applicable for the solving of environmental problems grow day by day. The different routes of synthesis of nanostructures have been developed and they reveal the high application potential in various fields. Particularly in the recent years zero valent iron nanoparticles ZVI NPs attract the significant interest as a soft reducing agent, and due to its biocompatibility it can be used in green environmental technologies. There are different synthetic procedures are developed for obtaining ZVI NPs. The excess amount of nitrates and chlorides has become serious problem of the water quality in farming sectors. Chlorides, Nitrates are potential harmful contaminants towards living organisms, and due to high solubility can easly pass and contaminate the earth and groundwater. Beside this among another most common environmental contaminants is chromium in its highest oxidation state Cr(VI). Cr(III) occurs naturally and is comparatively friendly towards environment, while Cr(VI) which has severe toxicity is generally released in environment from industrial processes, such as chromium mining electroplating, tannery facilities, metal fishing, and pigment manufacture.

In the present work the synthesis and characterization of zeolite and graphene oxide supported zero valent metall (ZVM), such as iron, nickel, cobalt nanoparticles (Ze-ZVM, GO-ZVM NPs) are reported. ZVM, Ze-ZVM and GO-ZVM NPs sizes, compositions and morphologies were characterized by Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Energy Dispersive Spectroscopy (EDS). Graphene oxide sheets have been used to prepare strong paper-like materials, membranes, thin films, and composite materials. Graphene oxide used as stabilizer and membrane component. Synthesized nanostructures were tested as reducing agents of nitrate and hexavalent Chromium. GO also was tested as membrane component for the removal of Cl^- ions. Batch experiments were carried for revealing of efficacy of prepared nanomaterials (ZE-ZVM NPs and GO-ZVM NPs). Nitrate removal efficiency (at initial concentration 50 mg/mL) was rapidly increased from 26% to 76% for GF-ZVI NPs at 60-240 min time interval for and from 34% to 90% for ZE-ZVI NPs at the same time interval. Also was studied the efficacy of prepared nanostructures ZE-ZVM and ZE-ZVM NPs as membrane component with 5% of ZVM NPS weight content for the removal of nitrate from water solution that made 85% for ZE-ZVM NPs and 95% for GO-ZVM respectively. The results of this study indicate that the application of grapene oxide GO-ZVM NPs, as membrane component is advantageous because it allows to prevent the additional pollution of treated solution caused by unreacted ZVM NPs. Zeolite and graphene oxide (GO) are inexpensive materials so they can be promising supporting materials for preparation of membrane component for removal of contaminates from water. Besides this the application of GO-ZVM and ZE-ZVM NPs as membrane component allow to prevent the additional pollution of treated solution with iron contaminates derived from ZVM NPs.

ENERGY STORAGE BY DECOMPOSITION OF INORGANIC SOLIDS – THERMOPHYSICAL PROPERTIES TO ASSESS REAL CYCLE PERFORMANCE

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Thermal dissociation reactions of inorganic solids are an interesting and cost-effective concept for the storage of thermal energy [1]. Nevertheless, the use of reversible chemical reactions for storing thermal energy is in a rather early stage of development. A potential reason is the time-consuming and costly experimental investigation of gas-solid-reactions. In this contribution, a general thermodynamic evaluation of reversible decomposition reactions is performed. Besides definite suggestions for efficient reaction systems, this study introduces a methodology for the identification of real storage performance with a minimized amount of input parameters.

The performed thermodynamic analysis can be split into two parts: 1.) Calculation of reaction equilibrium and investigation of the influence of thermodynamic driving force [2] at charging and discharging temperature. 2.) Performance of a comprehensive enthalpy balance including preheating of material, conversion and heat integration strategies. Both steps are necessary to determine potential operation temperatures, effective storage density and storage efficiency. Within the enthalpy balance, several scenarios for the operation of the thermochemical energy storage like fluidized bed and packed bed reactor, open and closed storage operation or short-term and long-term storage are taken into considerations.

All calculations are characterized by a minimum of necessary input parameters. Regarding the reaction equilibrium, thermodynamic driving force and enthalpy balance computation, enthalpy and entropy of formation as well as temperature-dependent specific heat capacities are needed. Furthermore, e.g. conversion, initial temperature of reactants and pinch temperature for internal heat recovery can be seen as free parameters and are varied in the modeling of the enthalpy balance in order to study the sensitivity of storage density and efficiency upon these variables.

The fundamental analysis identifies characteristic behaviors of all considered reaction schemes. Regarding the pressure-temperature-dependency of thermodynamic equilibrium, the correlation between ionic structure and thermochemical behavior is outlined. Furthermore, a method for the theoretical estimation of the necessary difference between charging and discharging temperature is developed and is successfully proven with data taken from literature [3]. Thus, based on the presented approach, the tendency of a reaction system to show high hysteresis is possible. The basis are the thermophysical substance properties. Thereby a thermodynamically sound preselection criterion could be developed. The calculation of the storage densities clarified that storage concepts, where the gaseous component is not released to the environment (closed concept), show quite low volumetric energy densities despite high enthalpies of reaction. Furthermore, the results prove that heat integration and heat recovery strategies are absolutely necessary in case of a long-term storage operation in order to reduce the energy demand for the preheating of reactants and to ensure a high efficiency. These results are used to prepare a comprehensive assessment matrix of all considered reaction schemes. It can be used for the material preselection as well as for the optimization of already investigated reaction systems.

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IMPACT BEHAVIOR OF NUGGET ZONE IN DISSIMILAR FRICTION STIR WELDED AA6061-T6 AND AA6061/SiCp COMPOSITE

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In this study, dissimilar friction stir welding (FSW) of AA6061-T6 and AA6061/SiC/20p composite that are hard to weld by most of the conventional fusion welding processes was investigated experimentally. FSW of the workpieces was carried out using a tool rotational speed of 1000 rpm, welding speed of 80 mm.min^{-1}, tilt angle of 1° and a penetration depth of 0.2 mm into the upper surface of the dissimilar sheets. A welding tool made from 4140 steel with a shoulder diameter of 20 mm and an unthreaded conical pin of 5 mm diameter was utilized during the process. In the present study, the monolithic alloy was fixed in the advancing side and single-pass welding procedure is performed. Temperature distribution around the weld zone was also measured during the FSW through a non-contact infrared thermometer (Fluke 576 CF) in order to check the maximum temperatures reached. Charpy v-notch impact tests of the joint were carried out so as to determine the impact toughness of the nugget zone of the weld. To this end, the Charpy impact specimens were prepared according to the standard (ASTM E23-04) and the impact tests were performed at room temperature using a pendulum-type impact test device. In addition, fracture surfaces of the impact tested specimens were investigated through a scanning electron microscope (SEM).

GLOBAL ASYMMETRY OF A NOVEL CONGRUENT VAPOR-LIQUID DIAGRAM PREDICTED FOR FLUID FULLERENES

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Development of molecular nanotechnologies needs the creation of universal predictive «tools» to study a fluid state diagram in usual molecular scales (from 0.1 to 1 nm) as well as within nanoscales (from 1 to 100 nm) of fullerenes. The fluctuational – thermodynamic (FT-) model proposed earlier by authors includes such main ingridients as: 1) the finite-range fluctuation Lennard-Jones (FLJ-) potential; 2) the global fluid asymmetry (GFA-) principle; 3) the congruent vapor-liquid (CVL-) diagram. The quite restricted experimental or simulated previously information just on a liquid state is necessary to predict CVL-diagram, to determine its stable part corresponding to the standard VLE- diagram and, at least, to estimate consistently the molecular parameters of FLJ-potential for further simulations and corroboration of predictions. The application of FT- methodology to the relevant problem of fullerenes, investigated until now mainly by the Girifalco potential, leads to the following preliminary conclusions. Both parameters of effective diameter and well depth are, most likely strongly overestimated for above standard potential selected for the solid state of fullerites. As a result, this situation may be the serious distortion factor at the simulation of VLE-diagram for C_{60}, C_{70}. Its striking asymmetry and the much wider range of stability have been revealed by FT-model. The main advantage of developed approach is a possibility to perform the thermodynamically-controllable one - phase simulations on the base of preliminarily predicted CVL- scetch. The further self - consistent procedure provides the testable and reliable prediction of the finalized CVL – diagram.

KEYWORDS: congruent, fullerenes, phase diagram.

ELASTICITY EXPANSIONS AND PREDICTION OF THERMODYNAMIC PARAMETERS UNDER HIGH PRESSURES

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We consider an approach to the evaluation of thermodynamic function of compressed liquids based on the general expansion of the elastic bulk modulus (the inverse is isothermal compressibility) $\kappa_{\mathrm{T}}^{-1} = (\rho/\rho_0)^n\left[\kappa_T^0 + \rho_0 k(P-P_0)\right]$, where the indices $n=-1,0,1$ correspond to the classic Tait equation, the Murnaghan equation, and the recently proposed [1] Fluctuation Theory-based Tait-like Equation of State (FT-EoS), respectively. The last one allows for predicting liquid's density under high pressures, as well as the isobaric expansivity, including such features as its isotherm intersection [1, 2], using the density and the isothermal compressibility data determined at normal pressure only.

On the other hand, it is found that the universal behaviour of the reduced density fluctuations, which assures such a predictive power, fails under extra high pressures corresponding to the percolation-like transition of molecular structure to the random dense packing [3]. In addition, there was an open question about possibility to calculate the speed of sound accurately without references to high pressure experimental data.

Here we show that the mentioned transition correspond to the change of index from $n=1$ to and $n=0$, and allows for connecting Murnaghan's parameter to the parameter k of FT-EoS. As a result, we obtained the predictive formula for the speed of sound under the elevated pressure P

$$c = c_0 + \left(\rho_0\kappa_{\mathrm{T}}^0\right)^{-1/2}\left\{\left[1+\left(\rho_0\kappa_{\mathrm{T}}^0\right)k\left(P-P_0\right)^{\frac{2\left(\rho_0\kappa_{\mathrm{T}}^0\right)}{\left(\rho_0\kappa_{\mathrm{T}}^0\right)-1}}\right]-1\right\},$$

which requires the knowledge of the reference (at normal pressure P_0) speed of sound, density, isothermal compressibility (can by expressed through the density, the speed of sound, and the isobaric heat capacity) and the coefficient k, which a function of two last quantities. In addition, the proposed approach provides more accurate results for the isothermal compressibility under high pressures, the internal pressure, etc., and clarifies reasoned structural basis for several previously known empirical dependences, e.g. Rao & Rao's rule, Kir'yakov's rule for the heat capacity ratio.

The derived predictive dependences are extensively tested on examples of a variety of organic liquids, from normal and halogenated hydrocarbons to ionic liquids, and the accuracy required for warrant technical applications, is confirmed.

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TRANSIENT HOT BRIDGE – A NEW METHOD TO MEASURE THERMOPHYSICAL PROPERTIES

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The thermal conductivity, temperature diffusivity and specific heat capacity are the most important parameters of new efficient materials for the energy and process technology.

The determination of these material properties requires various costly measuring devices and time-consuming measurements. With the newly developed and patented Transient Hot Bridge (THB), all three parameters can be determined simultaneously and within a few minutes. The Transient Hot Bridge is an absolute measuring method. No calibrating or reference measurement is required.

The Transient Hot Bridge covers a wide measuring range for thermal conductivity between 0.01 and 500 W / (m·K). Therefore, the THB is very well suited for determining the thermophysical properties of polymers, ceramic materials, construction and insulation materials, minerals and glasses, metals and alloys etc. The measurement uncertainties lie in the area of conventional plate or laser flash devices.

Sample preparation is very simple. In the case of solids, two sample halves with a planar surface are sufficient, between which the sensor is inserted. In the case of liquids, pasty samples or bulk solids, special measuring sensors are available, which can be inserted directly into the sample.

CONSISTENCY VERIFICATION OF EQUATIONS OF STATE

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In developing an equation of state (EOS), a general mathematic formulation is usually sought which describes the experimental data qualitatively well. Subsequently, this formulation is refined to a special formulation which predicts the data sufficiently accurately. In order to verify the EOS consistency, residuals, i. e. deviations between experimental and predicted values, are compared with their uncertainties. In verifying the consistency, it has not yet been taken into account how the scattering of individual experimental values affects the scattering of individual predicted values caused by fitting the EOS coefficients.

The methods for fitting alone, which are described in the literature, e. g. the least–squares method alone, are not sufficient to determine the correlation between experimental and predicted values.

In this presentation, a Monte Carlo method is introduced making it possible to describe the correlation with the Bravais–Pearson correlation coefficient. Starting out from fictitious experimental data, whereto the coefficients of different polynomials are fitted, it is shown that in verifying the consistency, considering correlation leads to rejection rather than non–considering.

It is therefore expected that the EOS consistency can be verified more reliably, if the correlation is taken into account. A consistent EOS prevents the accuracy of predicted values from being overestimated.

KEYWORDS: Data correlation, equations of state.

THERMOPHYSICAL PROPERTIES OF 1-ALKYL-3-METHYLIMIDAZOLIUM IONIC LIQUIDS WITH PF_6 ANION

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Ionic liquids (ILs) are a salt in the liquid form, which are very popular substances using in the industry during the last years. They are potentially "green" replacements for conventional organic solvents, because they have negligible vapor pressure, nonflammable, thermal stable, and recyclable properties. ILs are also claimed to be useful as heat transfer fluids in solar heating and absorption refrigerating systems, mass spectrometry, supports for the immobilization of enzymes, in separation technologies, as liquid crystals, templates for the synthesis of mesoporous, nano-materials and ordered films etc. Such wide range applications of them require high quality thermophysical properties, like as density, gas solubility, surface tensions, viscosity, diffusion coefficients, thermal and electrical conductivities.

This work is a continuation of our investigations in the field of (p,ρ,T) properties of ILs. The new accuracy (p,ρ,T) data of 1-butyl-; 1-hexyl- and 1-octyl-3-methylimidazolium ILs with PF_6 anions at the wide range of temperature T=(273.15 to 413.15) K and pressures up to p=140 MPa are reported with an estimated experimental relative combined standard uncertainty of $\Delta\rho/\rho$= ±(0.01 to 0.08) % in density, which were investigated using a Anton-Paar DMA HPM vibration-tube densimeter. The density measurements at ambient pressure were carried out using the Anton-Paar DSA 5000M density and sound of speed measurements. The heat capacities at ambient pressure and various temperatures were measured using the differential scanning calorimeter Pyris 1.

An empiric equation of state for fitting of the (p,ρ,T) data of ionic liquids with PF_6 anion has been developed as a function of pressure and temperature. This equation together with the heat capacity values was used for the calculation of the thermophysical properties of IL, such as isothermal compressibility $\kappa_T(p,T)$/MPa^{-1}, isobaric thermal expansibility $\alpha_p(p,T)$/K^{-1}, thermal pressure coefficient $\gamma(p,T)$/MPa·K^{-1}, internal pressure $p_{int}(p,T)$/MPa, specific heat capacities $c_p(p,T)$/J·kg^{-1}·K^{-1} and $c_V(p,T)$/J·kg^{-1}·K^{-1}, speed of sound $u(p,T)$/m·s^{-1}, isentropic expansibilities $\kappa_S(p,T)$ at high pressures and temperatures, in which the density of ILs with PF_6 were measured.

INVESTIGATION OF ACOUSTIC AND THERMOPHYSICAL PROPERTIES OF LIQUIDS BY ACOUSTIC PIEZOMETER METHOD

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Carrying out engineering and scientific calculations for the formation of scientific and industrial devices and for using them in technological processes requires high accuracy and reliability of experimental data on the physicochemical and thermophysical characteristics of substances. The ultrasound speed is one of the most informative parameters of the substance along with the density and isobaric heat capacity.

The acoustic method of research differs from other methods by its simplicity and reliability, but it has an accuracy, which is high enough. The acoustic method has a lot of variants.

The acoustic piezometer method allows to make p-ρ-T measurements and ultrasonic speed measurements simultaneously. The speed of sound was measured by the pulse method of one fixed distance, the density – by the bellows piezometer method.

The authors created a universal device comprising an electronic unit for generating, receiving and processing signals based on the programmable logic integrated circuit (PLIC) “Board DSP-310-2K” and a computer for measurements and calculations the acoustic, physicochemical and thermophysical characteristics of substances. This device replaces several bulky devices: a two-channel generator of rectangular pulses, a two-channel high-frequency amplifier, a frequency meter, an oscillograph, as well as decoupling and signal matching circuits, and allows to automate the measurement and calculation process.

The device allows to measure the ultrasonic speed as well as liquid density and to calculate the physicochemical and thermophysical characteristics of substances in automatic mode with high accuracy in a wide range of temperatures, pressures and ultrasound frequencies.

Calculations of physicochemical and thermophysical characteristics of substances were carried out using both well-known thermodynamic formulas and the formulas obtained by the authors within the cluster model.

The results of our measurements and calculations of the acoustic, physicochemical and thermophysical characteristics of the investigated liquids correlate with well-known experimental and calculated data.

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EVALUATION OF THE TRANSPORT PROPERTIES OF IONIC LIQUID-BASED ELECTROLYTES AS THE FUNCTION OF THE TEMPERATURE AND COMPOSITION

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Modified UNIFAC-VISCO [1-2] and UNIFAC-CONDUCTIVITY [3] group contribution methods were developed for the correlation and estimation of the transport properties of a series of pure ILs and their mixtures with molecular solvents as a function of temperature and composition at 0.1 MPa using a large set of recommended data from the literature. In this original approach, exemplified in Figure 1 in the case of the viscosity of pure ionic liquids, the salt (ionic liquids and/or molten salts) was divided into two peculiar function groups, cation and anion. Binary interaction parameters were determined by fitting the recommended experimental data and by minimizing the objective function. The transport properties of cations, anions, and salts showed an exponential behavior with the temperature well described thanks to the Vogel-Fulcher-Tamman (VFT) equation. Calculated VFT constants and binary interaction parameters were used to evaluate the viscosity, conductivity, diffusion coefficients and ionicity of selected electrolytes.

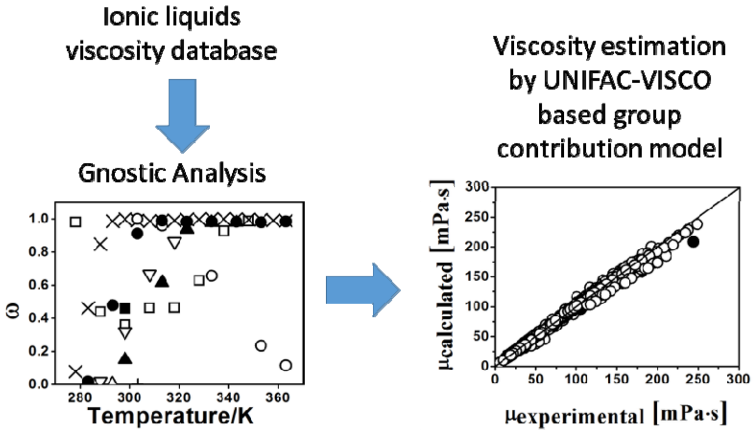

Figure 1: Methodology applied during this work.[2]

The estimation result showed a good agreement with experimental data with a relative absolute average deviation lower than 5 % in each case.[1-3] This novel approach will be presented and discussed in detail during this presentation.

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Poster Presentations

THERMOPHYSICAL PROPERTIES OF ZIRCONYL NAPHTHENATES SYNTHESIZED BASED ON NATURAL OIL ACIDS

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It is known, that catalytic systems consisting of zirconyl carboxylates obtained on the basis of differences carboxylic acids and alkyl aluminium chlorides widely have been using for oligomerization process of ethylene to linear higher α-olefins (C_4-C_{18}) [1,2]. Zirconyl naphthenates synthesized on the based of natural oil acids by us. The complex catalytic systems obtained by interaction of synthesized zirconyl complexes with aluminium organic compounds used in oligomerization process of ethylene to linear α-olefins. It was determined that catalytic systems obtained based on zirconyl naphthenates show higher catalytic activity in oligomerization process of ethylene to linear α-olefins. [3].

In this thesis were given the results of investigation of thermophysical properties of zirconyl naphtenates (MC1, MC2 and MC2) obtained basis on fraction of natural oil acids, separated from Baku oils boiling 5mm Hg at 120-130 °C, 160-180 °C and 187-197 °C. The DSC curves of the synthesized zirconyl naphthenates are given below.

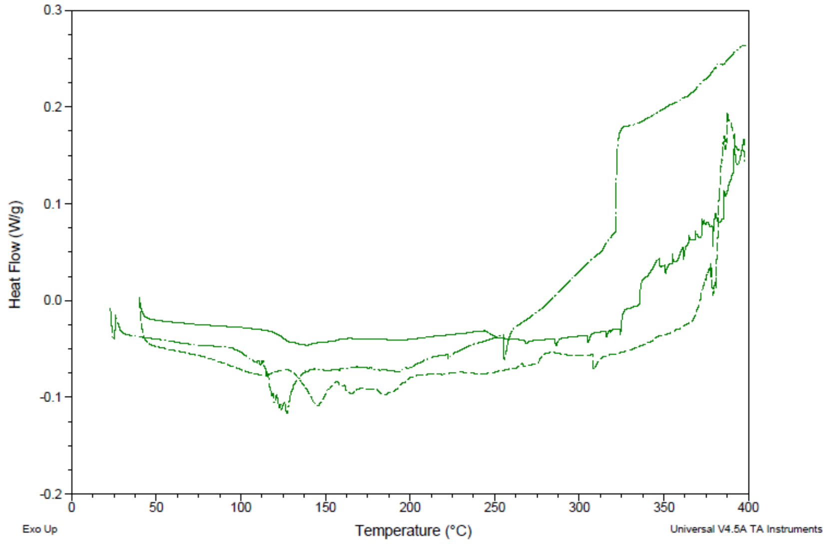

Figure: The DSC curves of MC1 (----), MC2 (—) and MC3 (—-) zirconyl naphthenates.

As can be seen the begining melting temperatures of these complexes are observed at 92-114 °C. The maximum temperature of observing endothermic peaks in the DSC curves are 127-145^0C and ending temperature of those are 140-162 °C. The entalphy of this process is ΔH=1.467 – 3.360 J/g. Thermal oxidation temperature of synthesized zirconyl naphthenates begin in the temperature interval of 194 – 205 °C.

Thus, as seen from DSC curves synthesized zirconyl naphthenates accordingly its thermophysical properties is suitable in oligomerization process of ethylene at low temperature as complex catalyst component.

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THE PERSPECTIVES FOR THE EFFICIENT USE OF THERMAL WATERS

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Thermal water, which is in natural conditions, can become too cold, and be cold, thermal, as well as overheated. Hot or geothermal water is not only the source of minerals, but also gives a person available and free geothermal energy. An important factor is the temperature of thermal water. Let’s mention an interesting fact – at great depths the water reaches the state of so-called “water plasma”. This state is characterized by the fact that on one hand, the water ceases to be water, and on the other hand, was not water steam. It occurs when due to high temperatures, the velocity of molecular motion is comparable with the speed of molecular motion of water steam, but the density remains in liquid state as in the water. Such steam-water mixture is often thrown out to the surface in the form of so-called Geysers. Depending on geothermal features of the region, there occurs a change in water temperature. It is the reflector of tectonic, age, hydrodynamic, as well as lithological features of water-bearing strata. The water temperature has a direct influence on the viscosity, filtration rate and also chemical composition and density. The change in density of pure water varies depending on the temperature 30 °C — 0,9839 g/cm^3 100 °C - 0,95838 g/cm^3. The water density depends on temperature, gases, dissolved salt, as well as suspended particle.

Scientific and experimental studies related to the solution of the problems on unconventional use of solar, wind and thermal water energy are carried out in many developed countries. The quality of thermal energy storage and high heat-and-power engineering volume of thermal water make them particularly important energy carrier.

Geothermal resources were first used in industry in Italy in 1904. Following Italy Geothermal power plants were built in New Zealand, Japan, the Philippines and the United States. So, today the first place on using thermal water takes Iceland. Geothermal energy is used in Finland, France, Belgium and Germany as well. In these countries, almost all settlements are heated by this energy. Despite the fact that the geothermal sources cannot completely cover all needs of a person, they are able to significantly reduce the need for use of natural fuel.

Thermal water is wide spread in the territory of Azerbaijan and it is used for different purposes. Forecast of useful thermal water storage in the republic is as follows: Southern slope of the Greater Caucasus – 2,000 m^3/day (30°C -50°C), Guba-Khachmaz zone – 21,000 m^3/day (40°C-70°C), Apsheron peninsula– 20,000 m^3/day (20°C-70°C), Mountainous part of the Lesser Caucasus – 4,000-5,000 m^3/day (30-74 °C), Nakhchivan AR – 3,000 m^3/day (40°C-53°C), Talysh mountain ragion – 15,000 m^3/day (31°C-43°C), Lenkoran plain – 7,000-8,000 m^3/day (44°C-64°C), Kur-Araz lowland – 170,000 m^3/day (22-95 °C), In republic – 245,000 m^3/day.

Comprehensive study of ecologically clean energy source of thermal water along with other types of fuel (mainly oil and gas) and use for the benefit of the people is a very important task.

KEYWORDS: Thermal water, fresh water, ecologically clean energy, temperature,

p,ρ,T,x - PROPERTIES OF WATER+ALCOHOL BINARY MIXTURES IN THE CRITICAL AND SUPERCRITICAL REGIONS

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P, ρ, T, x properties of binary water+methanol, water+ethanol, and water+1-propanol mixtures have been measured over a wide temperature and pressure ranges: from (373.15 to 573.15) K and densities between (10 and 600) kg·m^{-3} up to 40 MPa for three concentrations (0.2, 0.5, and 0.8 mole fraction of alcohol). These temperature and pressure ranges include one-phase (liquid and gas), two-phase, the critical and supercritical regions. The well-known high-temperature and high-pressure constant-volume piezometer technique was employed for the measurements. The measurements were concentrated in the critical and supercritical regions in order to study of the features of the mixtures critical curve behavior (critical phenomena in the aqueous alcohol solutions) and other derived thermodynamic properties near the liquid-gas critical points. The combined expanded uncertainty of the density (ρ), pressure (P), temperature (T), and concentration (x), measurements at the 95 % confidence level with a coverage factor of $k = 2$ is estimated to be 0.15 %, (0.02 to 0.05) %, 15 mK, and 0.01 mole %, respectively. The phase transition ($T_{\mathrm{S}} - P_S$ and $T_{\mathrm{S}} - \rho_S$) and critical curve data ($T_{\mathrm{C}} - x$), ($P_{\mathrm{C}} - x$), ($\rho_{\mathrm{C}} - x$), were determined from the measured $P\rho Tx$ properties. The measured values of $P\rho Tx$ were used to develop multiparametric equation of state

$$Z = p / RT\rho_m = 1 + \sum_{i=1}^{m} \sum_{j=0}^{n_i} a_{ij} \omega^i / \tau^j \ ,$$

where $\omega = \rho / \rho_C - 1$ and $\tau = T / T_C - 1$. Developed equation of state represents the present density measurements in the whole experimental range with an AAD of 1.4 % in the vapour phase and 1.0 % in the supercritical region. Saturated liquid and vapour densities were represented using scaling relation

$$\rho_{l,g} = \rho_C \left(1 \pm \mathrm{B}_0 \tau^{\beta_0} + \mathrm{B}_1 \tau^{\beta_1} \pm \mathrm{B}_2 \tau^{\beta_2} + \cdots\right),$$

where $\tau = \left(T_C - T\right) / T_C$, β_0, β_1, and β_2 are the universal critical exponents. The relative uncertainty of the saturated density representation is within (2 to 3) %. The shape of the critical curves was studied. For water + methanol and water+ethanol mixtures the critical curves are positively deviate from linearity, while for water+propanol mixture negative deviation from linearity was found.

MEASUREMENTS OF THE DENSITY, SPEED OF SOUND, VISCOSITY AND DERIVED THERMODYNAMIC PROPERTIES OF GEOTHERMAL FLUIDS FROM SOUTH RUSSIA GEOTHERMAL FIELD

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Density (ρ), speed of sound (W), and viscosity (η) of natural geothermal fluids from south Russia Geothermal Fields (Dagestan, Caspian seashore) have been measured over the temperature range from (277-353) K at atmospheric pressure. The measurements were made using the Anton Paar DMA4500 densimeter and Stabinger SVM3000 viscodensimeter for four geothermal fluid samples from the various hot-wells Izberbas (No. 68 and 129), Ternair (No. 27T and No. 38T). A sound-speed analyzer (Anton Paar DSA 5000) was used for simultaneously measurement of the speed of sound and density of the same geothermal fluid samples. The average differences between the measured geothermal fluids densities and viscosities and pure water values (IAPWS formulation) are within (0.1-1.77) % and (0.13-2.1) %, respectively, which are considerably higher than their experimental uncertainties. This differences are caused by the high concentrations of some type of ion species, such as (Na^+: 7.7 g/l (#38T); Cl^{-1}:7.7 g/l (#38T); SO_4^{-2} :0.75 g/l (#68); S^+: 0.24 g/l (#68); K^+:0.15 g/l (# 27T); Ca^{+2}:0.074 g/l (#27T); B^+:0.06 g/l (#38T); and Mg^{+2}: 0.033 g/l (#38T)), in the geothermal fluids, which strongly effect on salt concentration dependence of the measured properties. Measured values of density and speed of sound were used to calculate other derived thermodynamic properties such as adiabatic coefficient of bulk compressibility (β_S), coefficient of thermal expansion (α_P), thermal pressure coefficient (γ_V), isothermal coefficient of bulk compressibility (β_T), isochoric heat capacity (C_V), isobaric heat capacity (C_P), enthalpy difference (ΔH), partial pressure derivative of enthalpy $\left(\frac{\partial H}{\partial P}\right)_T$, and partial derivatives of internal energy (internal pressure) $\left(\frac{\partial U}{\partial V}\right)_T$, of the geothermal fluid samples. Measured values of density, viscosity, and speed of sound were used to develop correlation models for the temperature and ion species concentration dependences, which reproduced the measured values within 0.03% (density), 2.47% (viscosity), and 0.20% (speed of sound). To confirm the accuracy and predictive capability of the developed correlation models for density, speed of sound, and viscosity, we have applied the models to well-studied binary aqueous salt solutions (H_2O+NaCl). The prediction of the density and viscosity of aqueous sodium chloride solutions based on the developed models were very close to their experimental uncertainties (within 0.03% for density and 1.56% for viscosity). The measured properties at atmospheric pressure have been used as a reference data for prediction of the high-pressure thermodynamic behavior. The predictive capability of the model has been checked on reliable experimental data for binary aqueous NaCl solutions at high pressures reported by Kestin and Shankland (1984) and Rogers and Pitzer (1982). The prediction for density and viscosity is within 0.03% and 1.57%, respectively.

FUNDAMENTAL EQUATION OF STATE FOR BROMOBENZENE BASED ON A HYBRID DATASET

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A sufficient amount of reliable thermodynamic data is essential for the design and optimization of almost any process in the chemical industry. Fundamental equations of state (FEOS) are one solution for this problem, because they rationalize and summarize experimental data, offering a built-in interpolation and extrapolation scheme for general engineering purposes. The construction of a FEOS that covers the entire fluid region of industrial relevance typically faces the problem of scarce experimental input data. Molecular modeling and simulation have evolved to a point of acceptance in the applied sciences and are a potential solution to satisfy the need for thermodynamic data.

The experimental data situation for bromobenzene shows that it is a suitable fluid to apply the approach of fitting a FEOS on the basis of a hybrid dataset as introduced in [1]. This method is supported by the statistical mechanical formalism proposed in [2]. The formalism was designed to yield any derivative of the residual Helmholtz energy (for $x > 0$ or $y > 0$) $A^r_{xy} = \partial^{x+y}\alpha^r(T,\rho)/\partial(1/T)^x/\partial\rho^y \cdot (1/T)^x/\rho^y$ from a single molecular simulation run for a given state point, yielding exactly those derivatives that are required by the FEOS to calculate any thermodynamic property as a combination of these derivatives. In the present work, an extensive dataset was generated containing the six derivatives $A^r_{00}, A^r_{10}, A^r_{01}, A^r_{20}, A^r_{11}, A^r_{02}$, at 30 state points that are well distributed in the homogeneous fluid regions using the *NVT* Monte Carlo simulation.

In this work, an empirical fundamental equation of state correlation is presented for bromobenzene. The correlation is explicit in terms of the Helmholtz energy and it can be used to calculate all thermodynamic properties. The underlying dataset consists of experimental and molecular simulation data. The experimental data cover almost exclusively the gaseous phase and are available for temperatures from the triple point up to 473,15 K. Molecular simulation data are used to extend the validity to the liquid state and up to a maximum temperature of 800 K and a maximum pressure of 220 MPa.

The present FEOS correlation is explicit in terms of the Helmholtz energy α, which can be separated into an ideal gas part α^0 and a residual part α^r

$$\frac{a(\rho,T)}{RT} = \frac{a^0(\rho,T) + a^r(\rho,T)}{RT} = \alpha^0(\delta,\tau) + \alpha^r(\delta,\tau) \tag{1}$$

To describe the residual part of the reduced Helmholtz energy, an optimized functional form has been used:

$$\alpha^r(\tau,\delta) = \sum_{i=1}^{I} n_i \tau^{t_i} \delta^{d_i} + \sum_{i=I+1}^{K} n_i \tau^{t_i} \delta^{d_i} \exp(-\gamma\delta^{p_i}) \tag{2}$$

A nonlinear optimization procedure was used to develop Eq. 2. Because of the special data situation, the physical behavior of the FEOS in regions where no experimental data are available was carefully monitored. In the report the results of comparisons of calculated data on the Eq. 1 with the experimental and simulation data are presented.

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THERMOPHYSICAL PROPERTIES OF (OLIGO)ALKYLATE PRODUCTS OBTAINED IN THE PRESENCE OF IONIC LIQUIDS

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It is known that, recently, ionic liquids are being widely applied. Ionic liquids are currently of extensive interest as enabling environments, catalysts, solvents, etc. in many fields of science, including, organic chemistry, petrochemical, physical chemistry and other directions. It is known that alkylation is one of the processes which are carried out on the presence of ionic liquids.

The presented article is dedicated to studying thermophysical properties of products which were obtained from alkylation process of aromatic hydrocarbon (benzene, toluene, xylene) with α-olefins (hexene – 1, octene – 1, decene – 1). Data analysis was performed by Differential Scanning Calorimetry using DSC- Q -10 apparatus. DSC curves are shown in Fig. 1

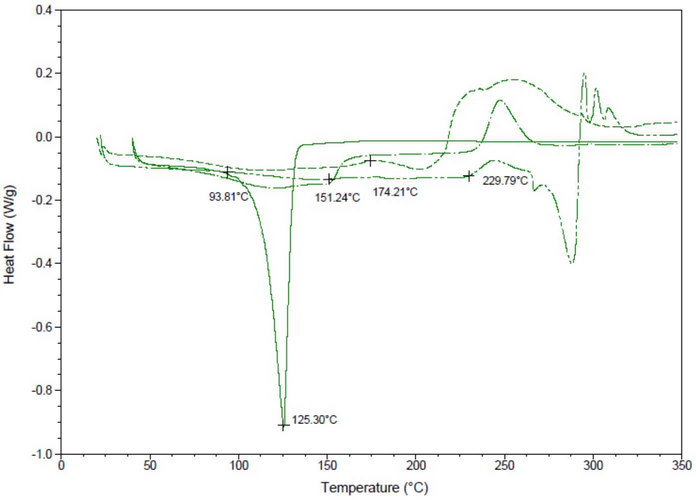

Figure 1. The DSC curves gasoline fraction from riforming process (___) and (oligo)alkylate products which were obtained in the presence of ionic liquid

It was shown that, beginning of boiling point of gasoline fraction which was obtained from riforming process is 93,81^{o}C, and the end of boiling is 151,24^{o}C. In this case the enthalpy is ΔH=59,03 J/g. But obtained products substantially differ from initial fraction as per their thermo physical parameters. So that their thermo-physical parameters appear after 180-200^{o}C. In lower limits of this temperature endothermic peaks with very small enthalpy (ΔH=2,36J/g) were observed. But thermooxidation destruction occurs at ≥200 ^{o}C and was observed with exothermic peak.

Thus, the obtained results once again prove that, ionic liquids are an effective catalytic system for alkylation processes. In the presence of this catalytic systems the thermooxidation stability of obtained products are high. In the future these products can be used as thermostable (oligo) alkylate materials.

THE THERMAL PROPERTIES OF n-BUTYL ETHERS OF HYBRIDIZED PHENOLFORMALDEHYDE OLIGOMERS

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It is known that one of the successful application of phenolformaldehyde oligomers is obtaining protective coatings, adhesive compositions on their base. Physico-mechanical properties of these compositions depend on their regulated curing. The purpose of the hybriding process of the resoles and novolacs is the obtaining of oligomers, which are characterized with wide keeping time, as the result of changes in the amount and location of functional groups (mainly methylol groups). The purpose of the etherification of the oligomers with n-butanol is conversion of methylol groups to large butoxy-groups, provision of non-polarity (for choise of non-polar solvents) and protective coatings on the basis of these indicators to have high adhesion and elasticity. The difference and advantages of n-butanol from other low and high molecular homologous alcohols have been identified in previous studies. As a result of the modification with nitrogenous compounds, the quality and performance improvement of oligomers have been proved. Therefore, the research work for the preparation of compositions on the base of n-butyl ethers of hybridized phenolformaldehyde oligomers and their nitrogen-containing analogues (on the basis of resoles and novolacs, modified with benzoguanamine) was carried out. These products differ from the original oligomers on following characteristics:

- in contrast to the resinous novolacs and resols, the viscous liquid form of the products eases their use, transportation and so on;
- the lack of viscosity, despite of the formation of larger macromolecules from the initial oligomers, can be explained by formation branced structures as well as linear structures;
- the synthesized oligomers have an extensive period of keeping for months and years to be suitable for application. This is connected with conversion of the functional groups, leading to the construction as result of intensive curing processes;
- these products have high physico-mechanical, sticky advantages as composition structure.

In order to learn of thermal destruction of n-butyl ethers of hybridized FFO, containing the different amount of various components thermoqravimetric analysis of samples at temperature up to 1000 °C, on the heating rate 10 °C/min and air flow has been implemented. As a standard, we used Al_2O_3. For the study, both the ordinary and the n-butyl esters of nitrogen-containing samples, hybridized in different mass ratios of novolac (one of the initial oligomers has been modified by the amount of 0,1-0,4 mol benzoguanamine on 1 mol phenol) and resole have been taken. The dramatic difference in thermal properties of oligomer samples were not observed, but in a general, we can put forward the following considerations: at 100-120 °C ~20% a loss of weight not accompanied by the rapid depolymerization. In this case endo-effects are observed, the solvent, alcohol, water allocation is assumed. The substantial destruction is began at the temperatures higher than 200 °C and 42-45% loss of weight at 200-280°C for n-butyl ethers of hybridized oligomers, obtained from resole, modified by the amount of 0,1-0,4 mol benzoguanamine on 1 mol phenol and novolac at their mass. ratio 2 : 1. The above-mentioned weight loss is registered at lower temperatures in the event of a modification of novolac (eg., at ~140-150 °C for n-butyl ethers of hybridized oligomers, obtained from resole and novolac, modified by the amount of 0,2 mol benzoguanamine on 1 mol phenol at their mass. ratio 2 : 1), while in the case of nitrogen absence oligomer at 210-240 °C more weight loss - 51,7-54,5% was observed. There is a poor growth on the further increase in temperature, the range of ~410-500 °C weight loss is 51-53%. 62-70% of the samples are subjected to destruction at 540-580 °C. At temperatures up to 1000 °C the oligomers decompose 98-100% or oxidate.

A sharp differences on oligomers of various component and the amount compositions were not observed in samples, and the following was revealed: a) in case of the amount of resole in hybridized oligomer; b) in case of increase amount of benzoguanamine in the range of 0,1-0,4 mol on 1 mol phenol in the resole; c) in case of modify of resole by benzoguanamine in hybridized oligomer compared to analoguos of modify of novolac, thermal resistance of oligomers are higher.

THERMODYNAMIC PROPERTIES OF SOLID SOLUTIONS OF REDOX-ISOMERIC O-SEMIQUINONIC COBALT COMPLEXES

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Redox-isomerism phenomenon is of great interest during last three decades due to possible application in molecular devices. o-Semiquinonic complexes of cobalt exhibit a redox-isomerism, i.e. the ability to exist in two forms differing by valent and spin state of metal and ligands. It was shown that the conversion of redox isomers is accompanied by phase transition.

Phase transition of o-semiquinonic cobalt complexes with 2,2’-dipyridil (2,2’-bpy)Co(3,6-DBSQ)$_2$ (**1**) and 1,10-phenanthroline (1,10-phen)Co(3,6-DBSQ)$_2$ (**2**) were quantitatively characterized [1, 2]. Complexes **1** and **2** are isomorphous and form solid solutions one in another with any ratio. Each solid solution reveals phase transition which follows redox-isomeric transformation upon temperature change. Thermodynamic parameters of phase transitions depend on the composition of solid solution. The heat capacity of solid solution (1:1) was studied in the range 7–350 K in an adiabatic vacuum calorimeter and the other ones were investigated by differential scanning calorimetry.

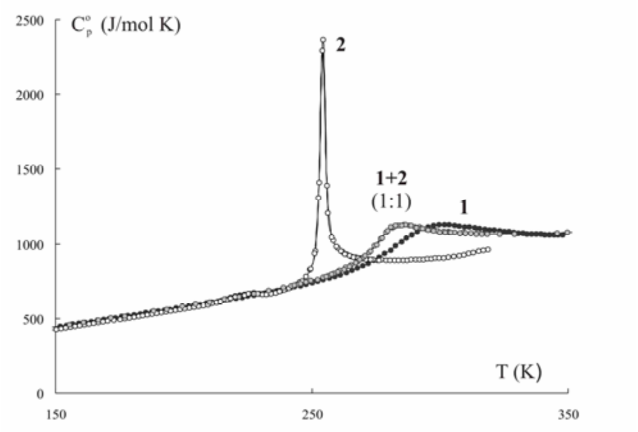

Fig.1 Heat capacity of complexes **1** and **2** and solid solution (1:1)

Resulting diagrams “transition temperature – composition”, “enthalpy – composition” allow us to evaluate the reciprocal influence of isomorphic lattices belonging to different redox-isomeric complexes.

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DESIGN OF A JOINT ON A CHIP

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In this study, an organ on a chip that would be an in vitro model for testing of next generation pharmacologic, tissue engineering, gene therapy and nanobiotechnological treatments was designed. It is an inevitable global necessity to develop this platform for safety tests of scientific studies in the field of medical technologies. Many researchers are working on this subject not only in our country but also in the most of the developed world. On the other hand, Orthopedics is another field becoming more and more important with increased average lifetime. Moreover, osteoarthritis and osteoporosis are affecting people’s life more dramatically. For this reason, tissue engineering, gene therapy and nanobiotechnologic approaches are developing to create new treatments for these diseases. Furthermore, a functional bone-joint organ on a chip, which includes all the fragments of joint including bone, bone marrow, cartilage and synovia, will be a scientifically novel and an answer to the demand of this scientific necessity. This study consists of design and modeling of a microfluidics device; design of nanotecnological or nano doped 3-D tissue scaffolds.

THERMODYNAMIC PROPERTIES OF TETRAGIDROALYUMINATE AND GEKSAGIDROALYUMINATE OF STRONTIUM

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It is known from the literature that the thermal decomposition process of tetra and geksagidroalyuminates of elements of groups IA and IIA proceeds in three steps as follows:

$$M(AlH_4)_{n(\text{тв})} = \frac{1}{3} M_3(AlH_6)_{n(\text{тв})} + Al_{(T)} + H_{2(\text{газ})} \tag{1}$$

by forming geksagidroalyuminates by scheme

$$M(AlH_6)_{n(T)} = MH_{n(T)} + Al_{(T)} + H_{2(\text{г})} \tag{2}$$

and the next step corresponds to a binary hydride thermolysis

$$MH_{n(T)} = M_{(\text{ж})} + \frac{n}{2} H_{2(\text{г})} \tag{3}$$

for borohydrides elements IA and IIA groups proposed the following scheme thermolysis

$$M(BH_4)_{n(T)} = MH_{n(T)} + nB_{(T)} + \frac{3}{2} nH_{2(\text{г})} \tag{4}$$

at a certain temperature in parallel with the scheme (4.) is a binary hydride thermolysis

$$MH_{(T)} = M_{(\text{ж})} + \frac{1}{2} H_{2(\text{г})} \tag{5}$$

We conducted selectively tensimetric research under equilibrium conditions for this purpose. It is known that complex tetragidroalyuminates of group IIA elements are formed in a solvated form synthesis conditions. We used desolvated original samples obtained directly in the cell membrane in our work. Non-solvated tetragidroalyuminat strontium $Sr(AlH_4)_2$ resulting in a membrane chamber was subjected to a further thermal decomposition. The experiment showed that the thermolysis $Sr(AlH_4)_2$ begins at 380K. The results of the study are given in Table 1.

The experimental data presented in the form, are well described by the equation

$$\lg P,_{\text{атм}} = (5{,}02 \pm 0{,}08) - \frac{(2{,}38 \pm 0{,}05)}{T} \cdot 10^3$$

in the temperature range (380-540) К.

The hydrogen pressure during the thermolysis of $Sr(AlH_4)_2$

T,К	P, кПа	T,К	P, кПа	T,К	P, кПа	T,К	P, кПа
I experience							
358	4	408	40	443	130	483	241
383	28	429	112	464	185	499	270
II experience							
405	11	444	169	205	374	508	538
423	38	453	203	220	505	533	623

According to this equation, was calculated the thermodynamic characteristics process of thermolysis $Sr(AlH_4)_2$, which is equal to ΔH^0_T=91,3±3 kJ·mol^{-1} and ΔS^0_T=192,1±5 J·mol^{-1}К$^{-1}$

Geksagidroalyuminate strontium. Over the completion of the thermolysis tetragidroalyuminate strontium, as evidenced by the shift in the barogram gas expansion line. After removing gas from the membrane and its heat at temperatures above 610K, there is pressure caused by thermolysis geksagidroalyuminate strontium.

The results of research of this process are given in Table 2.

The hydrogen pressure during the thermolysis of $Sr_3(AlH_6)_2$

T, К	P, мм.рт.ст.	T	P	T	P	T	P
I experience							
573	7	612	20	633	33	673	83
593	12	623	25				
II experience							
651	34	683	65	713	143	725	186
						743	291

The experimental data presented in the form $\lg P_{H_2} = f\left(\frac{1}{T}\right)$ described by the equation

$$\lg P_{H_2,\text{атм}} = (7{,}03 \pm 0{,}08) - \frac{(5{,}64 \pm 0{,}05)}{T} \cdot 10^3$$

in the temperature range (610-750) K. According to this equation the thermodynamic functions of thermolysis $Sr_3(AlH_6)_2$ was defined, which equal to ΔH^0_T=323,0±3 kJ·mol^{-1} and ΔS^0_T=404,0±5 kJ·mol^{-1}К$^{-1}$.

TAILORING IONIC LIQUIDS AS SOLVENTS BY COSMO-RS QUANTUM CHEMICAL METHOD

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Recently, due to development of modern science and technology the intensification of chemistry, organic synthesis, catalysis and other processes is required [1]. For development of this trend, there are a number of theoretical methods (GCMs, Monte Carlo, Schrödinger equation, Hartree-Fock and post Hartree-Fock methods, etc.) and computational programs (ADF, Gaussian, Octopus, MOPAC, Dmol3 etc.). It is possible to solve partially some ecological problems, improve economic efficiency and cost –effectiveness and eliminate the time waste by predicting processes using these methods.

Recently, intensive research works carried out on synthesis of ecological beneficial ionic-liquids and their application in various scientific fields including petrochemical and organic synthesis [2]. It is very important and promising to determine thermodynamic properties of ionic-liquid based processes and studying reaction mechanism. COSMO-RS method is more convenient and accurate for pre-forecasting ionic-liquid based processes including extraction, alkylation, etherification, oligomerization and polymerization [3].

Presented investigation includes the choice of various cation and anion containing ionic liquids as solvent for various hydrocarbons. It have been theoretically synthesized more than 200 ionic liquids and determined their various thermodynamic properties. Mutual solubility between ionic-liquids and aliphatic, aromatic hydrocarbons, N-, S-, O-containing compounds (cyclic acids, asphaltenes), simple ethers, especially alkyl-tert-alkyl esters was screened and analyzed [4]. The solubility of aforementioned compounds in ionic liquids determined due to aromatics capacity and activity coefficient.

As a result suitable ionic liquids were recommended for selective separation of aromatic hydrocarbons from Baku crude oil distillates. For example, asphaltene molecules which contains in oil distillates was screened. It was determined that two peak ($-0{,}6 \cdot 10^{-2}$ [e/A^2] and $0{,}3 \cdot 10^{-2}$ [e/A^2]) which observed asphaltenes sigma-profile doesn’t covered by n-undecane sigma profile. This fact showed that asphaltenes are not soluble in aliphatic hydrocarbons and it is possible to remove them from oil distillates with high selectivity. On the other hand, it was determined that ionic liquids peak observed in $-0{,}6 \cdot 10^{-2}$ [e/A^2] can not cover asphaltenes appropriate peak because it is very tall. It indicates that, there is partially wan-der-vaals interaction between ionic liqud and asphaltene molecule.

The next researches were about carbon dioxide solubility in various ionic liquids. Also, it has been determined appropriate thermodynamic properties for selective separation of alkyl-tert-alkyl ether, alcohol and hydrocarbon mixture.

Thus, it was determined that COSMO-RS method has great potential for researches on ionic liquids and obtained theoretical results are in good agreement with experimental data.

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THERMODYNAMIC PROPERTIES FOR MODELING THE INTERNAL COMBUSTION ENGINE *(WITH CASES OF APPLICATION)*

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When analysing or simulating technical processes thermodynamic properties are the basis to describe the gaseous, liquid or solid media. The same applies to analysing or modelling the combustion process in an internal combustion engine, which is one of the main topics of the chair of Technical Thermodynamics.

One of the main tools to analyse the combustion process of measurement data generated at the engine test bed is the in-cylinder pressure analysis. The inverse way is modelling the combustion process in a simulation tool to predict the engines working cycle. On the one hand there is the evaluation of measurement data, as mentioned e.g. in the in-cylinder pressure analysis, and on the other hand side there is the field of engine modelling for simulation and process evaluation. Both have in common that thermodynamic properties are needed with the following media, which has to be described: The intake air, the premixed or direct injected fuel that is mixed together with the intake air and as a product of the combustion process the exhaust gas. Handling those three mentioned pathways thermodynamic properties, especially caloric data, are used to describe the inner energy of the medium.

The presented publication will describe available approaches for the description of the mentioned media by using thermodynamic properties and will show where, in addition to it, further more data would be suitable. Finally, two exemplary current project will be presented as a case of application.

The first introduced project which will be shown is named “MEmBran” (Modelling of emissions and fuel consumption). Therein, the issue of ships manoeuvring is addressed meaning its transient operation behaviour. As the two main parts, experimental data of reference manoeuvring are investigated and an engine model is developed. Besides in-cylinder pressure analysis of measurement data, a ship’s main engine and powertrain model to predict efficiency and emissions is included. For the low dimensional modelling of the in-cylinder process thermodynamic properties are used. Furthermore, for the prediction of emissions reaction kinetic data are necessary.

The second project which will be presented is the simulation part of the LEDF (Low Emission Dual Fuel)-Project. This includes the modelling approaches of the thermophysical properties of gaseous fuels and the flame properties (ignition delay and laminar flame speed) at different thermodynamic conditions.

The publication will also include a summary and an outlook which future steps are necessary to improve the thermodynamic models to describe and model the in-cylinder process of internal combustion engines.

SYNTHESIS AND INVESTIGATION OF SOME NEW PHENOTHINSINE DERIVATIVES

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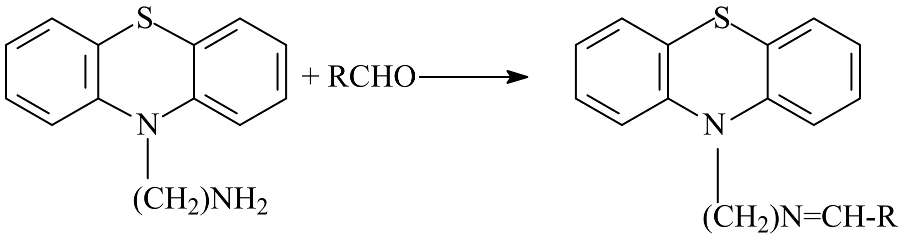
Phenothinsine drugs exhibit a wide range of biological effects. From the last few decades this chess of compounds attracted considerable amount of attention due to their different pharmacological activities [1] N-substituted phenothinsine are used widely in modern medical practice as neuroleptic, antipsychotic, antiurrhythmic medicines; Promethasne (Neyroleptic, antihistamine), chlorpromasine (antipsychotic), Triflurperusine (antipsychotic), Morucisine (antiurrhythmic).

Exhibition of promising antibacterial, anticancer, antiural, anti-inflammatory, antimalurial, trypanocidal, analgesic activities of new phenothinsine derivutives has been reported in literature [2] inspired by the mentioned achievements we have synthesized some N-sutstituted phenothinsine [3]. The structure-activity relationship of obtained compounds initially has been investigated.

By using 1,2-aminoalcohols as alkyluting reagents the officient methods of the new derivatives of N-substituted phenothinsine were elaborated:



Structure of the synthesized compounds has been confirmed by İR, ^{1}H. ^{13}C, NMR spectroscopy and elemental analysis. Synthesized compounds have been tested for antimicrobial activity, also as antioxidant, antiwear for lubricant oils.

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VISCOSITY MEASUREMENT OF THREE IONIC LIQUIDS AT AMBIENT PRESSURE

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Accurate viscosity data of ionic liquids (ILs) are required in order to study their suitability as several kind of applications, such us lubricants, hydraulic and thermal fluids, among others. This property depends strongly on their pressure and temperature conditions as well as their molecular structure. Thus, several viscosity values for these fluids ranging? At least from (6 to 7600) mPa·s at 298.15 K and 0.1 MPa were published [1]. It is important to remark that viscosity, as well as other thermophysical properties, is strongly dependent on the impurities, as water and halides [2].

In this work new viscosity measurements from 278.15 K to 313.15 K at atmospheric pressure for three ILs are presented. The viscosity of the 3 ILs, 1-ethyl-3-methylimidazolium ethylsulfate ($[C_2C_1Im][C_2SO_4]$), 1-butyl-3-methylpyridinium bis(trifluoromethylsulfonyl) imide ($[C_4C_1Pyr][NTf_2]$) and butyltrimethylammonium bis(trifluoromethylsulfonyl)imide ($[N_{4,1,1,1}][NTf_2]$), were measured by using two different devices. The first one is a vibrating-wire viscometer, which has been implemented at the Laboratory of Thermophysical Properties & Environmental Processes in Greece [3]. This device designed in such a way that allows absolute measurements of high-viscosity liquids in the temperature range (250 – 400) K and at pressures up to 30 MPa with an absolute uncertainty of ± 1.5 %. For the viscosity measurements of the ILs the electrical conductivity of the samples were taken into account in order to avoid alternative path of the current into the fluid. The second device is an Anton Paar Stabinger SVM3000 rotating cylinder viscometer located at the Laboratory of Thermophysical Properties in Spain [4]. This device was used to measure both the viscosity and the density of the 3 ILs with an uncertainty of 1% and 0.05%, respectively.

ACKNOWLEDGMENTS

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REFERENCE CORRELATION OF THE THERMAL CONDUCTIVITY OF 1-PROPANOL FROM THE TRIPLE POINT TO 600 K AND UP TO 100 MPa

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1-Propanol is one of the technically important substances and accurate information on its transport properties is desired for many applications. The data of thermal conductivity of 1-propanol is necessary for the calculation of the production processes, technological equipment, transport pipeline systems and so on. The use of 1-propanol in industry has made it one of the most important substances for which the development of accurate equations of thermal conductivity is needed.

Based on the most reliable experimental data, the equation for calculation of thermal conductivity of 1-propanol has been developed. The thermal conductivity of 1-propanol are expressed in this work using the equation

$$\lambda(\rho, T) = \lambda^0(T) + \lambda^r(\delta, \tau) + \lambda^c(\delta, \tau) \qquad (1)$$

where λ is the thermal conductivity in $\mathrm{mW \cdot m^{-1} \cdot K^{-1}}$, $\lambda^0(T)$ is the dilute gas thermal conductivity, $\lambda^r(\delta,\tau)$ is the residual fluid thermal conductivity, $\delta = \rho/\rho_c$; $t = T_c/T$; $\lambda^c(\delta,\tau)$ is the thermal conductivity critical enhancement. The dilute gas contribution is given by

$$\lambda^0(T) = N_1 \left[\frac{\eta^0(T)}{1 мкПа \cdot с} \right] + N_2 \tau^{t_2} + N_3 \tau^{t_3} \qquad (2)$$

where η0 is the dilute gas viscosity in mPa· s.
The residual contribution to the thermal conductivity is given (in $\mathrm{mW \cdot m^{-1} \cdot K^{-1}}$) by

$$\lambda^r(\delta, \tau) = \sum_{i=4}^{n} N_i \tau^{t_i} \delta^{d_i} \exp(-\delta^{l_i}) \qquad (3)$$

The thermal conductivity critical enhancement model of Olchowy and Sengers [Ref.] was used to calculate the fluid properties in the critical region.

The proposed equation can be applied over a temperature range from the triple point to 600 K with pressures up to 100 MPa. The equation was developed in variables «temperature-density» using a nonlinear optimization procedure. The report presents the results of the comparison with the available experimental data. In addition, the report presents diagrams that calculated based on the new equation. The diagrams are showing the good extrapolation behavior of the proposed equation. The proposed equation correctly reproduces the surface of state and allows the calculation of thermal conductivity with accuracy that is close to the experimental error.

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THE DENSITY OF N.BUTANOL + IZOOCTANE BINARY MIXTURES AT TEMPERATURES 298.15 to 550.15 K AND AT PRESSURES up to 70 MPa

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This paper deals with experimental results for the speed of sound in liquid binary n.butanol+izooctane mixtures and the calculation of thermodynamic properties at temperatures from 298.15 to 550.15 K and at pressures up to 70 MPa. The speed of sound has been obtained using a method of direct time measurement of an impulse traveling through the investigated medium in the temperature range 298.15-550.15 and pressure 0.1-70 MPa and concentrations 0-100 %. The pressure was measured by dead weight gauge manometers. The temperature was measured by platinum-resistance thermometer. Mixture composition was prepared by a weight method and was kept under control by chromatography analysis before and after measurements. The error of the experimental data does not exceed 0.06 %.

EXCESS AND APPRANET MOLAR PROPERTIES OF 1-ETHYL-3-METHYLIMIDAZOLIUM METHANESULFONATE AND METHANOL MIXTURES

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Ionic liquids and their organic solutions are successful claimed to be useful as heat transfer fluids in absorption refrigerating and solar heating systems, in separation technologies, as liquid crystals, templates for the synthesis of mesoporous, nano-materials and ordered films etc. Such wide interval of applications of ionic liquids requires high quality thermophysical properties. In this work, we will present the new (p,ρ,T) properties 1-ethyl-3-methylimidazolium methanesulfonate [EMIM][MeSO$_3$] and methanol mixtures at the wide range of temperature [T=(273.15 to 413.15) K] and pressures up to p=60 MPa with an estimated experimental relative combined standard uncertainty of $\Delta\rho/\rho$= ±(0.01 to 0.08) % in density, which were investigated using a Anton-Paar DMA HPM vibration-tube densimeter. Such wide range of measurements was carried out at the first time. The density of [EMIM][MeSO$_3$] and methanol mixtures at ambient pressure were measurements using the Anton-Paar DSA 5000 density and sound of speed measurements. The heat capacities at ambient pressure $c_p(p_0,T)$/J·kg^{-1}·K^{-1} and various temperatures were measured using the differential scanning calorimeter Pyris 1.

An empiric equation of state for fitting of the (p,ρ,T) data of [EMIM][MeSO$_3$] and methanol mixtures has been developed as a function of pressure and temperature. The properties of pure components were used during the developing of this equation of state. This equation was used for the calculation of the thermophysical, excess molar volume V_m^E/cm^3·mol^{-1} and apparent molar volume V^F/cm^3·mol^{-1} properties of the investigated mixtures.

CALORIC PROPERTIES OF DIMETHYL ETHER AND TRIETHYLENE GLYCOL SOLUTIONS

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The real working fluids of vapor compression refrigeration equipment are the solutions of refrigerants in compressor oils (ROS). Additives of compressor oil significantly affect the thermodynamic properties of the refrigerant and the energy efficiency of the compressor system. The optimum choice of working fluids is an important way to increase the efficiency of refrigeration equipment.

Prediction of thermodynamic properties of the ROS is difficult for several reasons. Firstly, there is no information on the composition of the compressor oil. Secondly, there is only a small amount of available information in the literature on the critical (pseudocritical) parameters for the thermally unstable compressor oils. These difficulties can be avoided by studying of the «model» thermodynamic systems that simulate properties of the ROS.

The main requirements to the «model» substance that simulate properties of the compressor oil are following: the availability of information about critical parameters; low values of the vapor pressure in the range of operating parameters of the refrigerating equipment; high molecular weight which can be found in the literature; unlimited miscibility with the refrigerant over a wide temperature range. In this report, we experimentally investigate the solution of dimethyl ether (DME), CAS №115-10-6 in triethylene glycol (TEG), CAS №112-27-6, which fully satisfies for the requirements listed above.

Caloric properties of the working fluids determine the efficiency of technological refrigeration processes. However, currently published methods to predict the heat capacity of refrigerant / compressor oil solutions are insufficiently developed and require further improvement.

New experimental data for the heat capacity on the saturation line for TEG, DME and DME/TEG solutions have been reported. Investigation of the two-phase region heat capacity was carried out on the experimental setup that realizes method of direct heating in adiabatic calorimeter. Experimental data for the heat capacity for pure DME, TEG and DME/TEG solutions in temperature range from 152 to 324 K at mass fractions of DME 20.85 %, 23.98 %, 24.53 %, 50.69 %, 50.91 %, 74.64 %, 74.69 % was obtained. The analysis shows that the mean uncertainty of the experimental data for the two-phase region heat capacity does not exceed 0.75 %. The data of isochoric heat capacity on the liquid saturation line, saturation heat capacity, isobaric heat capacity on the liquid saturation line, enthalpy and entropy for pure DME, TEG and DME/TEG solutions was obtained using the information on the two-phase region isochoric heat capacity. The methodology for predicting the caloric properties of ROS was developed. The influence of compressor oil additives on the caloric properties of DME and the efficiency of the compressor system has been studied.

STUDY OF SURFACE ROUGHNESS INFLUENCE ON DIRECTIONAL TOTAL THERMAL POWER RADIATED BY NICKEL

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Influence of surface roughness on thermal power radiated by materials at high temperatures was considered a lot of researchers [1,2]. However the influence of structure and height of roughness on the radiation was not studied experimentally. Our study is performed experimentally in the temperature range of 300-1100ºC in the air atmosphere. Nickel samples (Ni 99.9%) had isotropic and anisotropic rough surfaces. Diameter and thickness of the samples were 30 mm and 0.5 mm, respectively. The samples were heated by flat electrical heater and the thermal radiation of the samples passed through the cooled copper diaphragm having diameter of 12 mm. The passed radiation was received by the sensitive surface of the S302C sensor. The spectral range of the sensitivity was 0.19-20 μm for the sensor. Evolution of the sample surface during the heating was determined from diffraction patterns of probe laser light reflected by the surface. Dependences of the directional total thermal power radiated by the nickel samples on the height and structure of the surfaces determined experimentally are presented and discussed for the temperatures of 300ºC, 700ºC, and 1100ºC.

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ROLE OF STRUCTURAL VACANCIES IN PHYSICAL PROPERTIES OF GASB-GA$_2$TE$_3$ ALLOYS

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The presence of defects in the lattice, even in a small amount, has a significant effect on kinetic and thermodynamic parameters. From this point of view, solid solutions $(GaSb)_{3x}$ $(Ga2Te3)_{1-x}$, where the second component Ga_2Te_3 is a compound with a defective tetrahedral phase, are of definite scientific and practical interest. The Hall coefficient (R), electrical conductivity (σ), thermopower (α), and thermal conductivity (K) of the solid solutions have been studied as a function of composition 0 ÷ 5mol% Ga_2Te_3 and temperature (100÷550K). Synthesis of the samples was carried out in quartz cups placed in ampoules, evacuated to 0.01Pa with vibrational stirring. The samples were dense ingots consisting of several blocks, their number increased with increasing content of telluride in the alloy. The alloys had a zinc blende structure, the lattice constant decreased from 6.085 A for GaSb to 6.065A for the alloys with 10 mole% Ga2Te3, obeying Vegard's law.

Addition of the second component in GaSb (Fig.1) acts as a donor impurity, then the formation of a solid solution leads to appearance of a stoichiometric number of lattice vacancies acting as acceptors. The observed dependence of the Hall coefficient R (x) on the composition (Fig.1) is due to the successive transition of the process of substitution of antimony by tellurium (doping) to the substitution of tellurium by antimony with formation of cation vacancies and complexes that effectively scatter phonons, which leads to a strong decrease in thermal conductivity. This indicates the effectiveness of the use of these materials in thermoelectricity. The electrical conductivity (Fig.1) with a small addition of Ga_2Te_3 increases sharply, and then decreases monotonically. The dependences of α and K on the composition are shown in the Fig.2. According to calculations, the power factor $\alpha^2\sigma$ for 5mol% Ga_2Te_3 and at 300K is equal to 10μW/cmK^2.

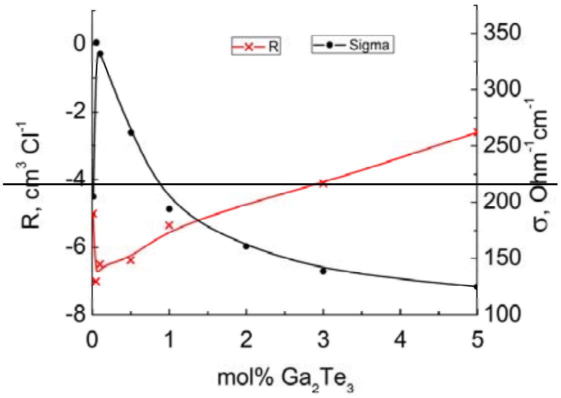

Fig. 1. Hall coefficient and electrical conductivity vs. of Ga_2Te_3 content

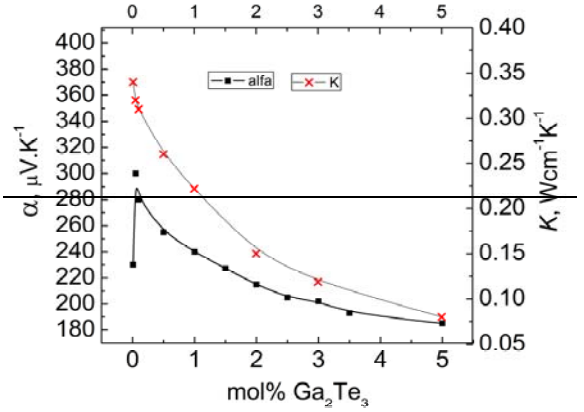

Fig.2. Thermopower and thermal conductivity vs. of Ga_2Te_3 content

EXPERIMENTAL INVESTIGATION OF THE VISCOSITY OF PROPYLENE GLICOLE BASED NANOFLUIDS WITH IMPROVED THERMOPHISICAL PROPERTIES

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An application of the heat transfer agents and coolants with nanoparticle additives is promising direction for intensification the heat transfer processes. The main advantage of the nanofluids for heat transfer application is their higher thermal conductivity compared to the base fluid. However, the main disadvantage of nanocoolants in comparison with base coolant is higher value of the viscosity.

The results of experimental investigation for the viscosity of the nanofluids based on aqueous solutions of propylene glycol and TiO_2 or Al_2O_3 nanoparticles are presented in this report.

Different technologies for the nanocooolants preparation based on two-step method have been analyzed in the report. Surfactants are not used at nanofluids preparation. As well known, the average size of the nanoparticles in the liquid determines its thermophysical properties. Thus, an assessment the degree of dispersion for the nanoparticles in nanofluids should be a preliminary stage during the experimental investigation of thermophysical properties and heat transfer processes. The mean size of nanoparticles in nanofluids that were prepared using different methods has been estimated. The evaluation of mean size for the nanoparticles in nanofluids was carried out by spectroturbdimetry method using spectrophotometer Shimadzu UV–120–02.

Measurements of the nanocoolant viscosity have been performed in the temperature range 248-293 K. Glass capillary suspended-level viscometer was used as a main part of experimental setup for measurements of the viscosity. The analysis of obtained results shows that an extended uncertainty for the kinematic viscosity does not exceed 0.035 mm^2/s. In addition, the nanofluids viscosity at different shear rates was examined using rotational viscometer.

The obtained results showed that method of the nanofluids preparation exercises significant influence on the mean nanoparticles size in liquid and on the viscosity of the nanofluids.

We also found that for particular systems the values of the relative viscosity (ratio between viscosity of the nanofluid and viscosity of the base fluid) are taken up smaller value at low temperatures (for some systems less than 1.0) compare to values at high temperatures (for temperature range 248 -293 K). This effect is undoubtedly important for the low-temperature heat transfer fluids. Even small value of TiO_2 or Al_2O_3 nanoparticle additives in solution of propylene glycol/water may improve its thermal conductivity. Corresponding increase the thermal conductivity of the solution together with insignificant increase of the viscosity contributes to enhancement the heat transfer processes in heat exchangers of the refrigeration systems.

Based on the obtained results the recommendations for choice of the optimal composition for coolants have been proposed. The method for predicting of the nanofluids viscosity in wide temperature range using minimum empirical information has been considered.

THE VISCOSITY BEHAVIOR AT THE GLASS TRANSITION PROCESS

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Molecular dynamics study [1,2] of shear viscosity behavior of liquid aluminum is performed. The embedded atom method potential is used at the simulation of isobaric cooling. The viscosity is calculated using the Green-Kubo formula.

The dependence of kinematic viscosity on temperature during the glass transition process is presented for different cooling rates [3]. The viscosity values above the melting temperature are close to the available experimental data [4]. The ensemble-averaged and time-averaged stress autocorrelation functions (SACFs) are obtained in the temperature range 300-1200 K. Study of the asymptotical behavior of the correlation functions and their peculiarities near the glass transition temperature is considered. Different glass transition criteria and the viscosity behavior are compared and related to the steep decrease of the decay exponent.

Also, the hysteresis of the transport coefficients is shown. The results are performed for cooling rates 2×10^{12} K/s and 4×10^{13} K/s. It is shown, that the more temperature of the transition grows as the cooling rate increase. That is in a good agreement with the results for structural and calorimetric criteria [5].

MD simulations of glass transition in a binary amorphous alloy is performed. The results for the liquid aluminum and the binary system are compared.

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LIBRARIES FOR CALCULATING THE PROPERTIES OF WORKING FLUIDS IN HEAT CYCLES, TURBINES, HEAT PUMPS, AND REFRIGERATION PLANTS

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The presented program libraries for calculating the thermophysical properties of water and steam, combustion-gas mixtures, humid air, refrigerants, and other working fluids are designed for practical use by engineers who calculate heat cycles, steam or gas turbines, boilers, heat pumps, or other thermal or refrigeration plants. Using these libraries, thermodynamic properties, transport properties, thermodynamic derivatives and inverse functions can be calculated.

The following property libraries are being presented here: LibIF97 for water and steam, LibIF97_META for metastable steam, LibICE for water ice, LibSeaWa for seawater, LibHuGas for humid combustion-gas mixtures also at high pressures, LibHuAir for humid air also at high temperatures and pressures, LibAmWa for ammonia/water mixtures in absorption processes and the Kalina process, LibWaLi for water/lithium bromide mixtures in absorption processes, LibIDGAS for combustion-gas mixtures, LibIdGasMix for 25 ideal gases and their mixtures, LibRealAir for real dry air, LibCO_2 for carbon dioxide including dry ice, LibNH_3 for ammonia, LibR134a for the refrigerant R134a, LibPropane for propane, LibButane_Iso and LibButane_n for isobutane and n-butane, LibD_4, LibD_5, LibD_6, LibMDM, LibMD_2M, LibMD_3M, LibMD_4M, and LibMM for siloxanes used as ORC working fluids, LibC_2H_5OH for ethanol, LibCH_3OH for methanol, LibH_2 for hydrogen, LibN_2 for nitrogen, and LibHe for helium. In addition, property libraries for a number of hydrocarbons are available.

These libraries contain the most accurate algorithms currently available for calculating thermodynamic and transport properties.

For extremely fast property computations in CFD and computationally intensive process simulations, spline-based property libraries for water and steam based on IAPWS-IF97 and IAPWS-95 are available. For other fluids, such property libraries can be prepared on request.

The presented property libraries can be used in user-specific programs written in Fortran, C++, C#, Java, Pascal (Delphi), Python, Visual Basic or other programming languages under Windows, Unix/Linux, or Mac OS.

In addition, add-ons for the use of these property libraries in Excel®, MATLAB®, Mathcad®, Engineering Equation Solver® (EES), Dymola® and SimulationX® (Modelica), and LabVIEW™ are available.

FAST AND ACCURATE CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES WITH THE SPLINE-BASED TABLE LOOK-UP METHOD (SBTL)

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The optimization of non-stationary processes in power plants and their components with heat-cycle calculation software, Computational Fluid Dynamics (CFD), and real-time process simulations require accurate and extremely fast algorithms for computing the thermodynamic and transport properties of the applied working fluids.

To fulfil these requirements, the Spline Based Table Look-up Method (SBTL) has been developed in a project from the International Association for the Properties of Water and Steam (IAPWS). This method has been applied to the Industrial Formulation IAPWS-IF97 and the Scientific Formulation IAPWS-95 for the thermodynamic properties of water and steam and the latest IAPWS formulations for the transport properties. SBTL functions of specific volume and specific internal energy (v,u), as well as of pressure and specific enthalpy (p,h) have been generated. With these functions, thermodynamic and transport properties, as well as their derivatives, are calculable in the single-phase region and in the two-phase region. Furthermore, numerically consistent inverse functions of pressure and specific volume (p,v) and specific internal energy and specific entropy (u,s) are obtained from the (v,u) SBTL functions. Analogously, inverse functions of pressure and temperature (p,T), pressure and specific entropy (p,s), and specific enthalpy and specific entropy (h,s) are obtained from the (p,h) SBTL functions. The properties calculated from the SBTL functions are in agreement with those of IAPWS-IF97 or IAPWS-95 within a maximum relative deviation of 10 to 100 ppm depending on the property and the range of state. In the single-phase region, computations from the (v,u) spline functions are between 130 and 470 times faster than those from IAPWS-IF97 and are between 240 and 430 times faster than calculations with IAPWS-95. The (p,h) spline functions are between 3 and 30 times faster than calculations with IAPWS-IF97 and are more than 6000 times faster than calculations with IAPWS-95.

The SBTL method has been successfully applied in several process simulation tools. In KRAWAL, the heat-cycle design software of SIEMENS, the overall computing time is reduced by 50% with regard to calculations based on IAPWS-IF97. In RELAP-7, the leading nuclear reactor system safety analysis software of the Idaho National Laboratory (INL), the simplified property calculation algorithms have been replaced with much more accurate SBTL functions. In the German Aerospace Agency's (DLR) CFD software, TRACE, the computing times for flow simulations of steam turbine stages are reduced by a factor of 10 in comparison to those based on the direct application of IAPWS-IF97. The numerical results of all these process simulations show negligible differences from those obtained through the direct application of the underlying property formulations.

For generating spline functions for fluid property calculations, the software FluidSplines has been developed. This software enables the application of the SBTL method to all kinds of property functions.

The developed method is the subject of the "IAPWS Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)".

SYNTHESIS AND INVESTIGATION OF SOME NEW 1,2-AMINOTHIOLY DERIVATIVE'S

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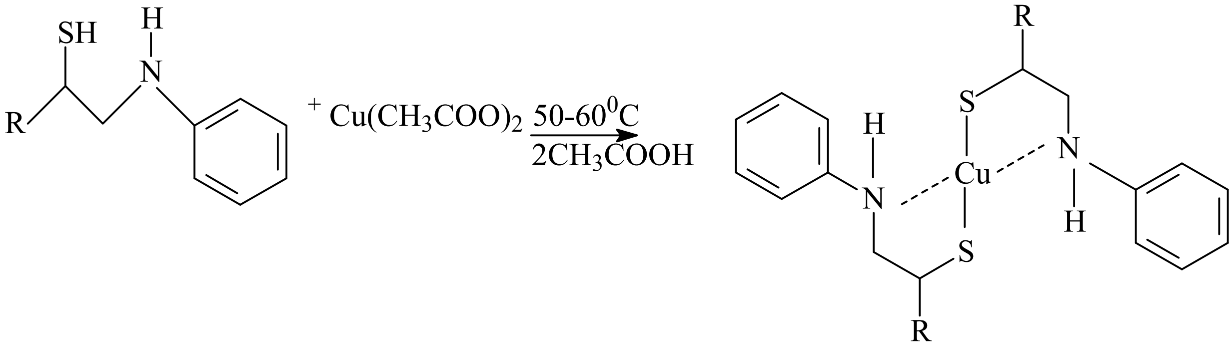
In the present study, the we have synthesized new alkyl-substituted 1,2-aminothiols through interaction of some thiiranes with aniline [1]. Although metalthiolutes have been knouwn since the beginning of co-ordination chemistry an attractiny biological importance and the numerous potential applications, and also from structural point of view. Therefore by the interaction of 1,2-aminothiols with Fe, Co, Ni, Cu acetates new complexes of the title compounds have been obtained.



R=CH_3; OCH_3

Structure of the synthesized compounds have been investigated by modern physicochemical methods of analysis. The dependence of additives properties from their structure has been studied.

Synthesized compounds have been investigated as an antimicrobial, antioxidative, antiwear and antiscoring additives for lubricant oils it has been determined that of them exceed in quality the industrial additives “İonol”, “Anglomol-99”, and “X-oxiquinolin”.

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NOVEL METHODS OF SYNTHESIS OF CALCIUM CARBONATE NANOTUBES AND NANORODS

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Nanofibers are objects of extensive research since its anisotropic morphology causes anisotropic behavior. Nanorods could be defined as solid nanoparticles with the shape of rod while nanotubes of carbon and inorganic compounds with layered structure present a layer or a group of layers folded in one direction to form a “seamless” tube with typical diameters from one nanometer to few hundreds of nanometers and length from few hundred of nanometers to few tens of micrometers and wall thickness of molecular dimensions. Nanotubes of non-layered inorganic compounds present hollow cylinders made either from atoms or nanoparticles. Nanotubes of non-layered calcium carbonate may present interest for application in drug delivery because of the biocompatibility of calcium carbonate and the structure which permits encapsulation of drug molecules. On the other hand since it was shown that nanoparticles of calcium carbonate improve properties of ordinary Portland cement with large amount of Supplementary Cementing Material (SCM) and also it is known that inorganic nanotubes have quite high Young’s moduli, it is suggested that nanotubes of calcium carbonate could also be applied for reinforcing cement with high concentration of SCM.

Since inorganic compounds with layered (2D) crystal structure are able to form nanotubes under certain conditions, in our research we have synthesized calcium carbonate nanorods and nanotubes basing on carbonation of calcium hydroxide nanotubes obtained in the first step. In two different syntheses two methods for synthesis of calcium hydroxide were used–solvothermal synthesis and solution phase synthesis with addition of polymer. In solvothermal synthesis carbonation was achieved by dissolving CO_2 in the solvent while in solution phase synthesis it was achieved by simple exposure of synthesized calcium hydroxide nanotubes to CO_2 in the air. Thus the solvothermal synthesis at 240°C with the molar ratio between solvent (ethylenediamine) and precursor (CaOHCl) of 360 carried out for 2 and 10 days gave nanofibers which are single nanorods of aragonite and bundles of aragonite nanotubes and nanorods with the average lengths of 1100±100 nm and 2600±400 nm correspondingly and diameter of 130±10 nm and 160±20 nm accordingly, while solution-phase synthesis with PEG gave nanotubes of $Ca(OH)_2$ and $CaCO_3{\cdot}6H_2O$ with length of around 300 nm and diameter of around 30 nm.
Although there were several reports on the synthesis of aragonite nanorods and one report on the synthesis of calcite nanotubes to the best of author’s knowledge there were no reports on synthesis of aragonite, $CaCO_3{\cdot}6H_2O$ and calcium hydroxide nanotubes by now. So this research suggests two methods for the synthesis of calcium hydroxide and calcium carbonate (aragonite and $CaCO_3{\cdot}6H_2O$) nanotubes and novel method for synthesis of aragonite nanorods.

THERMOPHYSICAL PROPERTIES OF CASPIAN SEA WATER

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The changing of climate and increasing of middle temperature in the Earth and Seawater surface, aslo speeding up evaporation of Sea water. The Caspian Sea is the largest lake on Earth with a surface area of 371,000 km^3 and a volume of 78,200 km^3. Depending on the inflow of fresh water from its rivers, the Caspian Sea is a freshwater lake in its northern portions. It is more saline on the Iranian shore. The largely dried-up Garabogazköl embayment approaches oceanic salinity. The region has very high temperature in the most time in year up to T=323.15 K and this fact play important role for the evaporation of water. In this case, the salinity of water is increasing. The nature around of Caspian Sea is dry and has much sand. The drink water resources are limited, ecpesially in the east coast. In this case, desalination of Caspian Sea water for drinking and domestic use is very actually in this region. The ship navigation (mostly oil and container tankers) is also most active in this region.

In this conference, we will present the (p,ρ,T) properties of the Caspian Sea water. The samples for the experiments were taken from various parts of the Caspian Sea. The experiments were carried out temperatures at T=(278.15 to 353.15) K and pressures up to p=40 MPa. The density measurements of the Caspian Sea water at the high pressures were carried out using the Anton-Paar DMA HPM vibration-tube densimeter. The salinity analysis of samples was carried out using the 8400B “Autosal” Laboratory Salinometer. The DMA 5000, DSA5000M densimeters were used for the density measurements at the atmospheric pressure and obtained results were compared with the (p,ρ,T) results extrapolated to p=0.101 MPa. An equation of state for the fitting of (p,ρ,T) properties of the Caspian Sea water was developed. The chemical analysis of samples (cations and anions) were analysed using the IRIS Intrepid II Optical Emission Spectrometer and DX 100 ion chromotography.

An empiric equation of state for fitting of the (p,ρ,T) data of the Caspian Sea water samples has been developed as a function of pressure, temperature and salinity of water. This equation is used for the calculation of the thermophysical properties of samples.

PHYSICAL PROPERTIES OF TERPHENYLS WITH RESPECT TO THEIR SUITABILITY AS LOHCS

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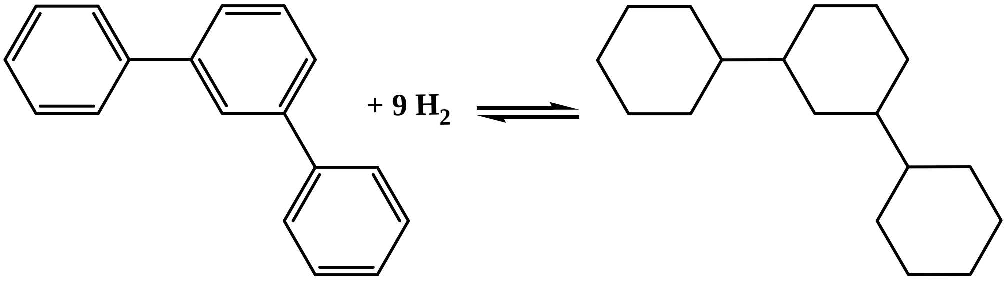
Liquid Organic Hydrogen Carrier (LOHC) are an interesting option for the storage of hydrogen through reversible hydrogenation of aromatic compounds. Terphenyls have emerged as a new potential class of materials in this respect.

Terphenyl usually consist of a mixture of three isomers, which can be hydrogenated reversibly to their respective saturated derivatives.



However, despite its promising chemical and thermodynamic properties its physical properties, especially its high melting point, is disadvantageous compared to conventional LOHC materials like dibenzyltoluene. Nevertheless, mixtures of isomers or with small amounts of other LOHC materials can achieve reasonable physical properties.

In this contribution, the feasibility of hydrogen storage using terphenyl as a LOHC is evaluated with respect to its physical properties. The focus is set on the effect on the ease of handling. Hence, important properties are melting point and viscosity. The properties are analyzed and compared to other LOHCs like N ethylcarbazole and dibenzyltoluene.

The authors wish to thank Prof. Wolfgang Arlt and Prof. Peter Wasserscheid for valuable discussion and Michael Geißelbrecht for the provision of samples.

ELECTRICAL MEASUREMENTS OF SiC/Au SCHOTTKY DIODE IN A WIDE TEMPERATURE RANGE

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Metal - semiconductor diodes (MSD‘s) play a favor role in constructing some useful devices in microelectronic, optoelectronic and semiconductor technology [1-2]. Some compound semiconductors with large band gap for example silicon carbide (SiC) has important properties such as thermal and chemical stability, oxidation resistance, high hardness and strength, etc. This material and diodes produced from this can be operate at high temperatures, high radiation environments and high power applications. The use of silicon carbide crystal has increased rapidly in recent years because of its potential applications.

In this study, 6H-SiC/Au Schottky barrier diode was produced. After chemical cleaning, Au is covered over the back side of the sample in 10^{-6} mbar pressure atmosphere with a thickness of 150 nm by metal evaporation method. Later it is annealed at 500 C for five minutes to form ohmic contact. For making of Schottky contacts, the metal Au of 150 nm thickness through a stainless steel mask of diameter 1 mm are deposited on the polished side of the n-6H-SiC wafer and the temperature dependent current-voltage (I-V) measured and analyzed in the temperature range of 80 - 400K. The I-V measurements were made with Keithly 2400 Sourcemeter by steps of 25 K. The barrier height and ideality factor are derived by using thermionic emission theory were found to be strongly temperature dependent. It was observed that the barrier height decreases and ideality factor increases with decreasing tempareture.

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PHASE DIAGRAMS OF HYDROCARBON MIXTURES FROM MOLECULAR SIMULATIONS: FORCEFIELD COMPARISON

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Molecular dynamics simulations are performed to calculate vapor-liquid equilibrium of methane-butane mixtures. Three models are tested: TraPPE-UA united-atom forcefield [1], OPLS-AA [2, 3] and TraPPE-EH [4] all-atom forcefields. The temperatures in the retrograde region of mixtures are considered.

The forcefields show good agreement with experimental vaporization curves of pure hydrocarbons. They also reproduce well the composition of liquid phase in binary mixtures as a function of pressure at isotherms, while significant discrepancies from experimental data are observed in the saturated vapor compositions with OPLS-AA and TraPPE-UA forcefields. The best agreement with the experimental phase diagram [5] is found with TraPPE-EH forcefield that accurately reproduces compositions of both liquid and vapor phase. This forcefield can be recommended for simulation of two-phase hydrocarbon systems.

The vaporization curved calculated with the TraPPE-EH forcefield are compared with the cubic equations of state [6] widely used for the description of hydrocarbon fluids. The accuracy of the molecular model is comparable to that of the cubic equations which allows us to use this forcefeld in future to provide input for cubic equation of state fitting procedure.

The effects of porosity on mixture phase diagram are qualitatively studied. The saturation curves in slit pores with Lennard-Jones walls are calculated. It is shown that nanopores may shift the coexistence curve. At certain wall-molecule interaction parameters, a significant widening of the pressure range of the retrograde condensation is found.

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CALORIC (C_V, V, T) AND THERMAL (P, V, T) PROPERTIES MEASUREMENTS OF PURE ISOPROPANOL AND ISOPROPANOL BASED NANOFLUID IN THE CRITICAL AND SUPERCRITICAL REGIONS

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Caloric (C_V, V, T) and thermal (P, V, T) properties of 2-propanol have been measured over a temperature range from (314 to 515) K for densities between (324 and 679) kg·m^{-3} and at pressures up to 8 MPa. The measurements were made in the single and two-phase regions in the immediate vicinity phase transition and critical points. From the measured values of saturated densities and vapor pressure data the values of the critical parameters ($T_C = 508.4\,\mathrm{K}$, $\rho_C = 273.0\,\mathrm{kg\cdot m^{-3}}$, and $P_C = 4.93\,\mathrm{MPa}$) were extracted. The measurements were performed using a high-temperature and high-pressure nearly constant volume piezo-calorimeter.

(C_V, V, T) and (P, V, T) properties of the nanofluid based on the 2-propanol and TiO_2 as a nanoparticles (15 nm in size) in the critical and supercritical regions were studied. The effect of nanoparticles concentration on the critical properties and phase transition behavior of pure 2-propanol was studied. The measurements were made for concentrations of nanoparticles from 0 to 20 wt %. The measurements of the isochoric heat capacity (C_V), *PVTx* properties, susceptibility (χ_T), order parameter ($\Delta\rho$), and the critical temperature for various concentration of nanoparticles (for $L_n << \xi$, where L_n is the characteristic distance between the nanoparticles and ξ is correlation radius, and for $L_n \to \infty$, ordinary pure bulk 2-propanol sample) were performed. The measured results were used to determine of the universal finite –size scaling functions and the effect of distance L_n between nanoparticals in the nanofluid on the properties near the critical point. We experimentally observed that the discontinuity (ordinary scaling power laws) that appears in the thermodynamic limits ($L_n \to \infty$) is smoothed for finite volumes ($L_n << \xi$). The crossover from bulk singular behavior ($L_n \to \infty$) of C_V and χ_T to finite-size behavior ($L_n << \xi$) was experimentally observed. We experimentally studied how measured isochoric heat capacity(C_V), susceptibility (χ), order parameter ($\Delta\rho$), and the critical temperature (T_C) vary as the average distance (L_n) between the dispersed nanoparticles in 2-proponal changes. This work was supported by the Grants of Russian Found of Basic Research №16-08-00536 and №15-08-01030.

THERMO-PHYSİCAL PROPERTİES OF ESTERIFICATION PRODUCTS OBTAİNED IN THE PRESENCE OF CATALYTIC SYSTEMS BASED ON THE NATURAL ZEOLITES

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The reactions of esterification are important for petrochemistry and organic synthesis. Products obtained in this way, including a number of simple and complex esters when added to fuels and lubricants as oxygenates, along with increasing fuel capacity, prevent the spread of noxious gases into the environment. The development of new heterogeneous catalysts for the reactions of esterification is an urgent problem.

The main goal of our work is to develop new and effective (nano)catalytic systems based on natural zeolites (clinoptilolite and mordenite type) of Azerbaijan for the reactions of (trans)esterification. The titanium oxide (IV) was used as a component of catalytic systems. Catalytic systems were prepared by a variety of physical and chemical means (precipitation, thermolysis, annealing, acid treatment, etc.). Number of acids and alcohols, isobutylene and some triglycerides were chosen as the components of the esterification reactions for synthesizing esters.

The resulting products were identified by a variety of physico-chemical methods (IR, NMR spectroscopy, gas chromatography-mass spectrometry, gel permeation chromatography, differential scanning calorimetry). The ways to regulate the thermophysical properties of the gained products depending on the number of (nano)metal particles and acid groups contained in the composition of the catalytic systems. The results were compared with the known catalytic systems and their impact mechanisms were also identified. Ways for regulation the thermophysical parameters of the products depending upon the nature of the active centers of the catalytic systems were analyzed. In the presence of these catalytic systems the thermooxidation stability (≥250°C) of obtained products are high. In the future these products can be used as thermostable fuel and lubricant components.

Thus, the studies hold promise for the development of new environmentally-friendly technologies based on natural raw materials.

VIBRATIONAL AND STRUCTURAL INVESTIGATIONS ON 7-HYDROXY-4-(TRIFLUOROMETHYL)-2H-CHROMEN-2-ONE

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In the present work, the quantum chemical calculations were performed by means of the Gaussian 09 software package, using hybrid density functional theory (DFT) at the B3LYP/6-311G (d,p) level of theory. All the computations have been carried out in gas phase. In order to establish the stable possible conformations, the conformational space of 7-Hydroxy-4-(trifluoromethyl)-2H-chromen-2-one molecule was scanned with theoretical methods. The harmonic vibrational frequencies have been calculated at the same level of theory. The vibrational frequencies were calculated and scaled, and subsequently values have been compared with the experimental Infrared and Raman spectra. The vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program. The observed and calculated frequencies are found to be in good agreement [1-3]. The Hirshfeld charge, fukui function and molecular docking analysis studies have been reported. Additionally, the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}) and the energy gap between E_{HOMO} and E_{LUMO} ($\Delta E_{HOMO-LUMO}$) have been calculated.

VIBRATIONAL (FT-IR, FT-RAMAN AND NMR SPECTRA) AND DFT ANALYSIS ON 5-[2-(TRIFLUOROMETHYL)PHENYL]FURFURAL

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Vibrational spectroscopy in combination with computational chemistry has been used systematically over the past decade to elucidate the spectroscopic, structures and some electronic properties of molecule. Various researchers used simulation methods such as DFT, HF simulations to explained molecular structure and vibrational spectra. Such study supports the experimental data in interpreting the calculations results of the structural and spectroscopic properties of the isolated molecule. The FT-IR, FT-Raman and NMR spectra of 5-[2-(Trifluoromethyl)-phenyl]furfural molecules have been recorded between 400-4000 cm-1 and 50-3500 cm-1 region respectively. The molecular geometry and vibrational frequencies of 5-[2-(Trifluoromethyl)phenyl]furfural molecules in the ground state have been calculated by using the Density Functional methods (B3LYP) with 6-311++ G(d,p) and 6-31G(d,p) as basis sets. The total energy distributions (TED) for the normal modes were computed for the minimum energy structure of the molecules. Comparison of the observed fundamental vibrational frequencies of 5-[2-(Trifluoromethyl)phenyl]furfural molecule with calculated results by density functional B3LYP approach will give better result for our studied molecular vibrational problem.

THE PRESSURE-DRIVEN DC CONDUCTION MECHANISMS IN POROUS MATERIALS

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Up to now, the structure and chemical composition of porous zeolite materials have been studied adequately, but there is insufficient knowledge about the physical properties associated with transport phenomena. This situation in particular is related to the electrical properties. The study of electrical conductivity, thermal electromotive force, dielectric permittivity and other parameters are important for the solution of a number of fundamental and applied problems of advanced porous materials. This is true when it comes to determining the activation energy, concentration and mobility of charge carriers, and the relaxation time. Electrical properties of natural zeolite, in practice have not been studied up to now. This is due to a number of objective difficulties namely; formation in nature in the form of small (0.1-0.01 mm to 1 μm) crystals, filling its cavities and channels by water molecules, the difference in the cation composition, the presence of phase boundaries and the presence of impurities [1]. It is necessary to identify the factors affecting the dc conductivity to improve the microelectro-optic applications of aluminosilicate materials [2]. Therefore, we study the bulk electrical conductivity of natural zeolites to understand the conduction mechanisms of the porous materials which is required to ensure proper optimization of gas discharge electronic device (GDED). Transport mechanisms were interpreted in details for GDED with zeolite cathode. It was shown that electronic conduction also contributes to ionic conduction which occurs in rare earth cations located in zeolites' inner structure, which occurs due to possible electron multiplication in pores and gas discharge gap. Thus, the main aim of our study was to show how pressure-driven new mixed electronic and ionic transport mechanisms of aluminosilicate materials occur when zeolite plates are used as a cathode in GDED.

The pressure-driven charge transport processes in microdischarges with a nanoporous zeolite cathode (ZC) are examined according to enhanced effect of electric field. The distributed resistance of the ZC and the impact of the ionizing component of the plasma on the control of the stable operation of a gas discharge electronic device at atmospheric pressure (AP) are investigated. The existence of water in the channels and pores is the decisive parameter in the ionic transport and it depends strongly on the electric field and gas pressure. When a high voltage was applied to gas discharge gap and porous structure, ionization phenomena increased. In this stage, electronic conduction also contributed to zeolite dc conduction. The contribution of charge carriers in conductivity varied in a wide pressure range up to AP air microplasmas in postbreakdown mode is discussed. The results show that the ionic transport predominated in low electric field while electronic transport predominated in the opposite conditions. Therefore, understanding of the ionic and electronic transport mechanisms of the porous materials are essential in enhancing applications in microdischarge devices with nanoporous ZC [3].

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THERMODYNAMIC PROPERTIES OF NANO FLUIDS IN DEPENDENCE TEMPERATURE AND PRESSURES

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The nanofluids are suspensions of solid nanoparticles with sizes typically of 1-100 nm in traditional liquid such as water, hydrazine, hydrazine hydrate, benzol and ethers. These solid-liquid composites are very stable and show a great enhancement in specific heat capacity and convective heat transfer with respect to traditional liquids and therefore they seem to be the “cooling medium of the future”. Nanofluids have been investigated recently to quantify the heat exchange performance, to identify the specific transport mechanisms and critical parameters and to develop specific production, management and measurement techniques. The experimental investigations include metallic nanoparticles (Cu, Al,Ti,Ni,Co,Ru, Ba, Fe, Au and Ag), oxide nanoparticles (CuO, Al_2O_3, TiO_2,BaO, Fe_2O_3,FeO_3 and SiO_2) and carbon nanotubes (CNTs) in traditional liquids such as water, hydrazine , hydrazine hydrate, benzoyl and ethers with a wide range of nanoparticle volume fraction and size. The experimental work carried out till now was not sufficiently systematic to collect a sound amount of coherent and unambiguous data with respect to methodology and results. However the experimental evidences show the possibility to apply successfully nanofluids as transport medium in several systems and processes. The experimental studies available in the up-to-date open literature on specific heat capacity and transport properties of nanofluids are focused mainly on the measurement of thermal conductivity and heat transfer coefficient, but the sets of data are quite widespread and cover the thermal range close to or above ambient temperature. The aim of this paper is to measure the thermal conductivity and the dynamic viscosity of (CuO, Al_2O_3, TiO_2,BaO, Fe_2O_3,FeO_3 and SiO_2) and carbon nanotubes (CNTs) nanofluid with a declared 10 nm average particle size and a nanoparticle volume fraction ranging from 0,1 to 0,5% in the temperature range from 0 to 100°C. The nanoparticles show a great tendency to agglomerate into clusters: the average cluster size measured by a DLS apparatus Malvern Zetasizer Nano ZS is around 105 nm, 10 time the declared average size of the dispersed nanoparticles. The experimental results were reported in term of absolute values and enhancement ratio with respect to the base fluid (water , hydrazine , hydrazine hydrate, benzoyl and ethers) at the same temperature The experimental measurements were also compared both with available measurements carried out by different researchers and classical computational models for thermodynamics properties of suspensions such as Maxwell’s correlations. All the classical models show weak ability to capture the experimental data and the discrepancy with measurement increases for increasing nanoparticle volume fraction.

THE THERMAL CONDUCTIVITY OF DIFLUOROMETHANE

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As a stratospherically safe refrigerant difluoromethane (R32) is considered as candidate to replace difluoromonochloromethane (R22) as a working fluid of HACR-technology. An experimental investigation of the thermal conductivity of difluoromethane in the critical region is presented. Thermal-conductivity data difluoromethane as a function of temperature and density was measured by a concentric-cylinder method in which a thin vertical fluid layer was subjected to stationary gradient imposed by heating the layer from interne coaxial cylinder. This method was realized for measuring the thermal conductivity in the vicinity of the critical point of R32. The geometrical configuration of vertical cell is the one where convection is to occur. To avoid laminar convection the gap between cylinders has been minimized and the applied temperature difference ΔT was chosen as small as possible. The limit for the convective heat transfer under these conditions and corresponding Rayleigh number are estimated. The thermal conductivity of difluoromethane in the critical region has been measured at densities up to 2.36 times the critical density and at temperatures from 356.63 K down to 294.72 K. The experimental accuracy was 2.5 to 10 % depending on the vicinity to the critical point. For the calculation of the densities and of the various thermodynamic properties was applied a new accurate equation of state. A new equation of state for R32 in the critical region that includes the scaling-low behavior of the thermodynamic properties is developed. Measurements in the high-density region indicate the critical-point thermal conductivity enhancement along isotherms in the researched temperature range.

THE MAXWELL FACTOR BEHAVIOR OF REFRIGERANT R32

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The thermal conductivity of refrigerant R32 has been investigated experimentally in a wide region temperatures, pressures and densities including the thermodynamic critical point. The purity of R32 is 99,84 %. The experimentally observed values of the thermal conductivity were used to examine the behavior of the Maxwell factor connecting the thermal conductivity, isochoric specific heat and the viscosity by the relation

$$\lambda = f\eta c_v$$

The coefficients f from the theory varies slightly with the temperature and for monoatomic gases $f = 2.5$. For polyatomic gases the value of f is lower and varies slightly with the temperature and density. The values of Maxwell factor of R32 in function of density and temperature were determined. The values specified heat at constant density c_v were obtained from the adopted in the work crossover equation of state. Presented equation of state was based on the phenomenological theory of critical point and Benedek’s hypothesis. The new equation of state was used to determine the thermodynamic properties of R32. The values of f observed for R32 including the critical region where the isochorique heat and thermal conductivity coefficient exhibits a sharp maximum are preserved. The Maxvell factor f R32 is practically independent of the temperature including the neighborhood of critical point.

THERMAL DIFFUSION OF HYDROFLUOROCARBON HFC-32 NEAR THE CRITICAL REGION

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The hydrofluorocarbon (difluoromethane, HFC-32) has been proposed as working fluid in refrigeration and air conditioning systems instead HCFC-22 prohibited after 2020 Year. The thermal diffusion values of HFC-32 were determined using a received cross-over equation of state and available experimental thermal-conductivity data reported by a number of investigations including the authors of this work. The quality of the received data on the thermal diffusion depend practically on the accuracy level of the experimental thermal-conductivity values and the specific heat at constant pressure.

Extensive measurements in this work have been obtained for thermal conductivity of difluoromethane with a steady-state method for which coaxial-cylinder apparatus was employed. The sample fluid was located in a narrow gap between two coaxial vertical cylinders. An amount of heat is generated through the fluid layer and in this way a temperature difference between cylinders is established. The occurrence of convection in the fluid was avoided one to application of small temperature differences across the gap.

The range of state points studied includes those with densities from 70 to 1000 $\text{kg}\cdot\text{m}^{-3}$, temperatures from 294 to 350 K and pressures up to 7 MPa. The isobaric specific heat values were determined from the crossover equation of state based on the phenomenological theory of a critical point and Benedek’s hypothesis. A theoretically based crossover model is capable to represent the thermodynamic properties of HFC-32 in a large range of temperatures and densities including the critical point.

The critical parameters of temperature, pressure and density of HFC-32 in the cross-over equation state has been adopted as the following values of T_c = 351.255 K, p_c = 5.78246 MPa, and ρ_c = 424 $\text{kg}\cdot\text{m}^{-3}$. A distinct «critical» minimum of thermal diffusivity was clearly observed at near-critical density.

THE RESEARCH OF BALAKHANI OIL BY USING NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

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The Balakhani oil which is produced in Absheron peninsula of Azerbaijan Republic has brown color and isostructures are relatively rich in its paraffin chain. The amount of aromatic hydrocarbons is very low for these oils (nearly 15%). The oil which has been chosen as a research object had a molecular mass of 284 g/mole, viscosity of 17.05 mm^2/sec in 20°C, density of 887.8 kg/m^3 and endpoint of boiling of 600°C. As a result of the research which has been done by NMR ^1H and ^{13}C methods, it has been revealed that the structure parameters of hydrocarbons those are separated from Balakhani oil by using different eluents (hexane, benzene, benzene-alcohol) and adsorbent (silicagel) have different values. The majority of hydrogen atoms in middle molecules (more than 90%) belongs to the saturated hydrocarbons.

The presented work has been dedicated to the research of the NMR – ^1H of aromatic and saturated hydrocarbons of Balakhani oil those are separated by adsorption method. The spectra of the samples were obtained with the Furye spectrometer with the frequency of 300.18 MHz from “Bruker” (Germany) at room temperature. Deuterium benzene has been used as a solvent. The relative portion of the protons those belong to different structure groups (aromatic, naphthene-paraffin and etc.) has been calculated according to the integrals of resonance adsorption stripe. Balakhani (fatty) oil and its hydrocarbon fractions those have been separated by adsorption have been investigated by the NMR – ^1H spectroscopy method and the parameters have been calculated.

The resonance signals for $–CH_3$ and $–CH_2$ groups have been observed in δ=0.88 and 1.28 ppm points. As it is clear from the table, the portion of the hydrogen atoms for these groups (H_δ and H_γ) predominates and generally, it is more than 46%. In naphthene structure, the portion of the protons are nearly 13% (δ=1.4–2.0 ppm), however for –CH–, CH_2– and CH_3 groups those are in α- position according to aromatic nucleus, it is nearly 5% (δ=2.0 – 2.9 ppm).

In order to investigate the saturated fragments in the “middle” molecules of fractions deeply, the proportion of the alkyl groups (CH_3 and CH_2) those are in β and γ positions according to the aromatic nucleus has been determined. It should be noted that, this ratio ($J=CH_3/CH_2$) is considered as a major parameter which characterizes the branching degree of aliphatic chain and called isoparaffin index.

The natural Balakhani oil and its naphthene – paraffin, 1st and 2nd group aromatic hydrocarbons those are separated by adsorption method are characterized by higher isoparaffin index (J, 0.50-0.46 according to the table). The high value of isoparaffin index proves the predominance of branched alkanes in the investigated well oil. For the other samples, (1st and 2nd group aromatic hydrocarbons and wax), the diversification of alkyl fragments is low, it changes around 0.4-0.3. That is why, the protion of the terminal methyl groups (H_γ) is not so high (overall 22-17%). The amount of the unsubstituted hydrogen atoms in the 2nd and 4th group aromatic hydrocarbons is 12%. The 1st and the 3rd group aromatic hydrocarbons and wax fractions are rich with saturated structures.

As a result of this research, it can be stated that the amount of the branched alkanes predominates in the investigated oil. This experimental fact gives a key to use the mentioned oil as a qualitative feedstock for catalytic cracking process.

Company Presentation

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Anton Paar GmbH is an Austrian company with its registered office in Graz that develops, produces and sells analytical instruments for laboratories and process analysis technology (PAT). It also supplies customised automation and robotics solutions. The company is specialised in the production of equipment for measuring density and concentration and in rheometry and the determination of dissolved carbon dioxide CO_2.

Anton Paar GmbH manufactures at its site in Graz and has five other manufacturing subsidiaries in Austria, Bosnia, Germany and Switzerland. Worldwide, there are 26 sales subsidiaries and numerous international sales partners.

The company Anton Paar is committed to long-term partnerships with customers and employees as well as responsibility towards society in general. Since 2003 Anton Paar has been owned by the charitable Santner Foundation. The foundation is exclusively and directly dedicated to charitable and beneficent causes.

Over 2500 employees at the headquarters in Graz and the 26 sales subsidiaries worldwide ensure that Anton Paar products live up to their excellent reputation. The core competence of Anton Paar – high-precision production – and close contact to the scientific community form the basis for the quality of Anton Paar's instruments.

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Dieckers is a member of the working group water jet technology (AWT) of the university of Hannover, which was founded in 1991 to develop applications for industries as well as for research and development. Actually there are 80 partners from nine countries that are members of the AWT.





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With more than 400 employees, more than EUR 60 million in annual turnover and eight foreign subsidiaries, LAUDA is the global leader in the manufacture of innovative thermostatic equipment and systems for science, application technology and production, as well as for high- quality measuring devices. With almost 60 years of experience and a unique product portfolio ranging from compact laboratory thermostats to industrial circulation chillers to customized heating and cooling system projects with more than 400 kilowatts of cooling power, LAUDA is the only company that can guarantee optimized temperature throughout the entire value-added chain for its 10,000 plus customers worldwide.

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Through numerous innovations and ongoing investment, LAUDA is sustainably improving its excellent market position and is growing both in the main European market as well as overseas.

LAUDA – The right temperature worldwide

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