

10th Rostocker International Conference Technical Thermodynamics Thermophysical Properties and Energy Systems



Book of Abstracts THERMAM 2021

10th Rostocker International Conference: **"Technical Thermodynamics:** Thermophysical Properties and Energy Systems"

Institute of Technical Thermodynamics

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BOOK OF ABSTRACTS

10th ROSTOCKER INTERNATIONAL CONFERENCE: "TECHNICAL THERMODYNAMICS: THERMOPHYSICAL PROPERTIES AND ENERGY SYSTEMS"

THERMAM 2021

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Preface

10th ROSTOCKER INTERNATIONAL CONFERENCE: "TECHNICAL THERMODYNAMICS: THERMOPHYSICAL PROPERTIES AND ENERGY SYSTEMS"

Thermodynamics is a very fascinating scientific field, which has to do with many different phenomena in nature and technology. 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 to a huge extend 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 within the atmosphere are governed by 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 thermodynamic problems knowledge of thermophysical properties is crucial. One example is the possible capture of carbon dioxide from raw biogas or exhaust gases in ionic liquids. To make this technically feasible, data on the thermophysical property of carbon dioxide solubility in the advanced material of ionic liquids are needed.

With 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 methods 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 propertie4s 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.

Even though the COVID-19 pandemia leads to this years THERMAM conference been held only online, this symposium will open many opportunities for scientific exchange. This new format will enable discussions in a new way, which might also show possibilities for the future.

We wish you all an interesting, pleasant and stimulating conference and hope to see you again next year next year at the 11th THERMAM conference in Rostock.

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Keynote Presentation

THERMODYNAMIC PROPERTIES OF CARRIER MATERIALS FOR HYDROGEN

Karsten MÜLLER

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Prof. Dr.-Ing. habil. Karsten MÜLLER is professor and chair of the institute of Technical Thermodynamics at the University of Rostock in Germany. He studied chemical engineering at the Technische Universtät München (Germany) and the University of Cape Town (South Africa). After graduating in 2009 he moved to the Friedrich-Alexander-Universität Erlangen-Nürnberg, where he received his PhD in 2013 for a thesis on CO₂ utilization. In 2018 he received is habilitation at the same university for his works on energy storage technologies. Before accepting the position as professor in Rostock, he conducted further research at the Pacific Northwest National Laboratory (USA) and the Forschungszentrum Jülich (Germany).



Hydrogen storage can benefit strongly from the utilization of carriers. For instance, Liquid Organic Hydrogen Carrier (LOHC) allow storing hydrogen in a dense and safe form. Chemical reaction with such a carrier material converts hydrogen in a liquid form that does neither require low temperatures nor high pressures. Hence, handling is simplified a lot and storage losses are avoided.

The thermochemical and thermophysical properties of the carrier materials have a tremendous impact on the performance of the storage process. Knowledge of these properties is required for two main tasks:

- 1. Design and optimization of the process
- 2. Control of the process.

Caloric properties like enthalpy and entropy of reaction (together with heat capacity) are not only needed to access heat demands or releases, but also govern the chemical reactions of hydrogenation and dehydrogenation through the reaction equilibrium. Furthermore, the performance of the reactors is strongly influenced by transport properties like viscosity and thermal conductivity.

Control of the process requires fast online determination of the degree of hydrogen loading of the LOHC. Correlation with thermophysical properties can help in this regard to reduce costs through simplification.

Understanding the effect of thermodynamic properties is therefore of utmost importance for the successful development of this technology. In this presentation, an overview will be given about the ongoing research on hydrogen storage technologies, which covers two aspects: Exact determination of the properties and understanding their impact on the overall process performance.

Plenary Presentation

BRINGING NEW MATERIALS INTO FUNCTIONAL ELECTRODES: PROSPECTS AND CHALLENGES

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Prof. Dr.-Ing. Doris SEGETS is professor at University of Duisburg-Essen. Her endeavour is the development of scalable formulation and coating technologies for nanomaterials applied in the field of energy conversion and storage, e.g. fuel cells and batteries. She received her PhD in 2013 from Friedrich-Alexander-Universität Erlangen Nürnberg (FAU) in the field of particle technology and was appointed as a professor for process technology for electrochemical functional materials at University of Duisburg-Essen (UDE) in 2018. In July 2020, she finished her habilitation in mechanical process engineering. Doris Segets' works are highly recognized (Friedrich-Löffler-Prize 2016, Dechema Prize 2020 and Gottschalk-Diederich-Baedecker Prize 2021). She is active within the community, e.g. as chairperson of the ProcessNet working group on interfacially dominated systems and processes, as member of the senate of the UDE and as member of the Young Academy of BBAW/Leopoldina.



New, micron and nano-sized functional materials play a key role for future technologies that are currently developed in the field of energy conversion (electrolysers, fuel cells) and storage (batteries). While new materials with outstanding properties are continuously developed by colleagues from chemistry and materials science, they rarely find their way into – urgently needed – large scale production and industrial applications. Overcoming and bridging this "valley of death" is an interdisciplinary endeavour for which chemical engineering and in particular, particle technology is indispensable. However, to fulfil this highly ambitious bridging function, the field needs to develop in such a way that we i) collect and make efficient use of more data and develop standard procedures that allow us to better understand process-structure and structure-property relationships, ii) replace idealized conditions and model formulations by technically relevant scenarios (testing at application concentration, full complexity of a formulation mixture) and iii) apply relevant processes (scalable dispersion, R2R-coating) already on lab-scale as integrating research tools.

ISOCHORIC HEAT CAPACITY AND PHASE TRANSITION PROPERTIES OF MAIN COMPONENTS OF BIOFUELS: METHYL DECANOATE

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Prof. Ilmutdin ABDULAGATOV is the chief of the Thermophysical division of the Geothermal and Renewal Energy Institute of the High Temperature Joint Institute of the RAS and chief of the Physical Chemistry Institute at the DSU, Makhachkala. Since 1998 to 2016, he appointed as researcher-professor at NIST in Boulder (Colorado, USA). He has more than 45 years expertise in the experimental study and modelling of the thermodynamic and transport properties of fluids and fluid mixtures at high-temperatures and high-pressures including the critical and supercritical regions. He is author more than 500 publications in peer-reviewed scientific journals, 12 books and book chapters. His publications focused to the thermophysical properties of fluids and fluid mixtures at high-temperatures at high-temperatures, phase equilibrium (VLE), heat-capacity, PVT, thermal conductivity, viscosity measurements of liquid and gases, including supercritical fluids and fluid mixtures, theoretically based scaling type of equation of state.



In the present work single – and two–phase isochoric heat capacity ($C_{v,\rho}$,T), and liquids-gas phase transition (T_{s} , ρ'_{s}) properties of methyl decanoate as one of the key biofuel's component have been studied. The measurements were performed along 15 liquid and vapor isochores between (152 and 834) kg·m⁻³ over a temperature range from (300 to 463) K at pressures up to 16 MPa using high-temperature and high-pressure nearly constant-volume adiabatic calorimeter. The combined expanded uncertainty of the density (ρ), temperature (T), and isochoric heat capacity (C_V) measurements at the 95 % confidence level with a coverage factor of k = 2 is estimated to be 0.15 %, 15 mK, and 3 %, respectively. For each experimental isochores the measurements were concentrated in the two-phase region in the immediate vicinity of the phase-transition temperatures (T_s) to precisely determine the phase boundary properties (ρ_s , T_s , C_{V1} and C_{V2}) using isochoric heat -capacity abrupt behavior technique. For ten liquid isochores of (731.8, 734.73, 752.59, 770.51, 786.10, 799.12, 804.15, 822.12, 828.56, and 834.82) kg·m-3 the phase transition temperatures (T_s) were experimentally determined using C_V discontinuity method (abrupt behavior of C_V). For other vapor (152.09 and 204.55) kg·m⁻³ and near-critical (235.13 and 300.83) kg·m⁻³ isochores we are never reached heat-capacity abrupt point temperatures (phase-transition temperatures, $T_{\rm s}$) due to thermal decomposition of the methyl decanoate at high temperatures (above 473 K), i.e., for these isochores the thermal decomposition of methyl decanoate occurs before reaching the phase transition temperature. The measured two-phase (Cv2) isochoric heat capacities as a function of specific volume (V) along the various isotherms (below 473 K) were used to accurately estimate the values of the second temperature derivatives of chemical

potential, $\frac{d^2 \mu}{dT^2}$, and vapor-pressure, $\frac{d^2 P_s}{dT^2}$, using theoretically based Yang-Yang relation. The contributions of the

vapors-pressure, $C_{VP} = VT \frac{d^2 P_S}{dT^2}$, and the chemical potential, $C_{V\mu} = -T \frac{d^2 \mu}{dT^2}$, heat capacities (theoretically meaning

properties) into the measured total two-phase C_{v2} of methyl decanoate were estimated. The measured two-phase heat capacity C_{v2} and phase boundary (ρ_s , T_s) property data were used to calculate the key thermodynamic property data (P_s , W_s , K_{TS} , C_{Ps} , ΔV_{LG} , ΔH_V , ΔS_V , ΔU_V , ΔC_V and ΔC_p of methyl decanoate along the saturation curve and the critical property data (T_c = 669.5±5 K and ρ_c = 287±5 kg·m⁻³).

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NOVEL TREATMENT METHOD TO REVERSIBLY CAPTURE AND SEPARATE CO₂ FROM SO₂ USING SUPERBASE IONIC LIQUIDS

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Dr. Johan JACQUEMIN has expertise in the development of in-house property databanks, the design of novel and original experimental apparatus and physical models able to predict properties with a view to understanding the physical and chemical nature of novel materials and design of viable chemical engineering processes. He passed with honours a PhD investigating thermodynamics of selected ionic liquids in July 2006 at the University Blaise Pascal (Clermont-Ferrand – France). He stayed for two years as Post-Doctoral Research Associate at Queen's University Belfast (QUB) in order to improve his knowledge of ionic liquids and more precisely their chemical engineering properties and applications. In September 2008, he joined the Tours University (France) as an Assistant Professor, and was involved in researching physical properties of novel materials (ionic liquids, electrolytes, solar cell materials) for use in battery and supercapacitor applications. Since, October 2017, he is an associate Professor in Thermodynamics at the Tours University and editor of the Journal of Solution Chemistry.



This talk will be focussed on recent results dealing with the utilisation of superbase ionic liquids (ILs) with a trihexyltetradecylphosphonium cation and a benzimidazolide ([P_{666 14}][Benzim]), or tetrazolide ([P_{666 14}][Tetz]) anion in a dual scrubber system for the reversible absorption of CO₂ and SO₂ under realistic conditions. In fact, we will clearly demonstrate that [P_{666 14}][Tetz] is capable of efficiently capturing SO₂ in preference to CO₂, and thus protecting [P_{666 14}][Benzim] from the negative effects of the highly acidic contaminant. Briefly, this results in [P_{666 14}][Benzim] maintaining > 53% of its original CO₂ uptake capacity after 30 absorption/desorption cycles, in comparison to the 89% decrease observed after only 11 cycles when [P_{666 14}][Tetz] is not present. Explanation of such a difference will be also explained during this talk thanks to an in depth characterization of the ILs carried out after exposure, revealing that small amounts of SO₂ are irreversibly absorbed to the [Benzim]- anion, which is responsible for the decrease in CO₂ capacity. This effect could be limited by solving engineering problems, presenting an opportunity to build on this feasibility study. The research, which will be shared during this talk, demonstrates that [P_{666 14}][Tetz] is a suitable sorbent for reversibly capturing SO₂, significantly extending the lifetime of [P₆₆₆ 14][Benzim] and maintaining a high CO₂ uptake capacity.

KEYWORDS: lonic liquids; CO₂ capture; SO₂; flue gas; scrubber.

THERMOPHYSICAL PROPERTIES OF ETHANOL + GASOLINE FUEL BLENDS AT HIGH PRESSURES AND OVER A WIDE RANGE OF TEMPERATURES

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Dr. Javid SAFAROV graduated with honours, received his PhD in 1993 and worked as research co-worker 1993-2005 years at the Azerbaijan Technical University. He worked at the University of Erlangen-Nürnberg of Germany in 2005-2006 years and since 2006 he is research co-worker at the institute "Technical Thermodynamics" of University of Rostock. He is member of the German group of the International Association for the Properties of Water and Steam (IAPWS), has honoured the Alexander von Humboldt (2003-2004, 2007) and Japan Society for the Promotion of Science JSPS (2004) fellowships. Dr. Javid Safarov is the co-author of 1 book, 2 monograph, 4 lecture book and more than 450 publications in the journals and conferences. He is leader of the research group of "Thermophysical properties of fluids" and specialist in the research field of investigations of the thermophysical properties of fluids at high pressures and wide range of temperatures.



Alternative fuel sources have received increased attention during the last decades due to worldwide environmental concerns, increasing of traditional fuel price and their expected depletion. Alcohols have been proposed as an alternative fuel sources to conventional fossil gasoline fuels and their usage strongly increased during the last years. Ethanol can be combined with gasoline because of its simple chemical structure, high octane number and oxygen content, and accelerated flame propagation. Thus, it is important to have reliable knowledge of the thermophysical properties of such fuel blends, such as density, vapor pressure, viscosity, speed of sound, heat capacity etc. which allows modeling, understanding, and optimizing the injection and combustion processes in an internal combustion engine.

This work presents analysis of various thermophysical properties of gasoline + ethanol binary fuel blends at temperatures T = (263.15 to 468.15) K, pressures up to p = 140 MPa and at volume concentrations $w_V = (0 \text{ to } 100) \%$. The (p, ρ, T) properties of these blends were determined using a high pressure – high temperature Anton-Paar DMA HMP vibrating tube densimeter. The observed repeatability of the density measurements at temperatures T = (263.15 to 468.15) K and pressures up to p = 140 MPa was within $\Delta \rho/\rho = \pm (0.01 \text{ to } 0.03) \%$. Additionally, heat capacity at temperatures T = (253.15 to 468.15) K, ambient and saturated pressures were measured using a differential scanning calorimeters ($\Delta c_p/c_p = \pm 0.5 \%$). The viscosity at p = 0.101 MPa and at temperatures T = (253.15 to 313.15) K were studied using an Anton Paar SVM 3000 Stabinger ($\Delta \eta/\eta = \pm 0.35 \%$) viscometer. The speed of sound at p = 0.101 MPa and at temperatures T = (278.15 to 323.15) K were measured using an Anton Paar DSA 5000 density and sound velocity meter ($\Delta u/u = \pm 0.1 \%$). An equation of state for fitting the (p, ρ, T) data of the investigated systems has been developed as a function of pressure, temperature and concentration. The various thermophysical properties of these fuel blends and excess molar volumes V_m^E were calculated at high pressures and temperatures, in which the (p, ρ, T) properties were studied experimentally.

Oral Presentations

REVEALING THE MELTING ENTHALPY OF CHOLINE CHLORIDE FROM THE SOLID-LIQUID EQUILIBRIA DATA IN ITS MIXTURES WITH COFORMERS

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Deep eutectic solvents (DES) are a new class of designer solvents prepared by mixing two or more components that form a eutectic mixture with significant negative deviation from ideal behavior. DES can be prepared by mixing different hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD). Knowledge of solid–liquid equilibria (SLE) is essential to the design of eutectic mixtures.

Choline chloride (ChCl) is the most widely used HBA in DES. So far, the reason behind the unique character of ChCl to form eutectic mixtures with a large depression in the melting temperature of the mixture at the eutectic point is not well understood. Based on SLE thermodynamics, the significant depression in the melting temperature of the mixture can be due to substantial negative deviation from ideality or low melting enthalpy values of ChCl. As ChCl decomposes before melting at around 575 K, it is impossible to measure its melting properties and adequately model SLE of ChCl containing DES.

In this work, we propose a new approach to determine the melting enthalpy of ChCl. The method is based on indirect estimation of melting enthalpy from the measured SLE data for the ChCl/coformer mixtures using activity coefficient model. The model parameters were estimated from the SLE data on the cocrystal melting properties and coformer-rich region. The melting properties of the cocrystals and the SLE of the two binary eutectic systems were measured using differential scanning calorimetry. The formation of ChCl cocrystals was monitored using powder X-ray diffraction (XRD), and the crystal structures were solved by single-crystal XRD. The measured liquidus temperatures of ChCl in each system and the activity coefficients of ChCl calculated using the NRTL model were used to estimate its melting enthalpy. The obtained melting enthalpy allows for a good description for the SLE data of both systems in contrast to previously estimated ChCl melting enthalpy values found in the literature. Generally, the proposed approach can be used to estimate the melting properties of the melting properties of the MBAs.

THE USE OF CLINOPTILOLITE AND GO FOR WATER PURIFICATION

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The zeolites have specific physical and chemical properties such as: intense ion exchange and selectivity, reversible hydration and dehydration, high gas absorption capacity, high temperature stability, resistance to aggressive media. The role of zeolite nanoparticles and graphene oxide in the treatment of water was studied. Clinoptilolite type of zeolite was used as a zeolite nanoparticle. The components contained in clinoptilolite are shown in the given table.

Table 1. The components of Zeolite type of Clinoptilolite.								
Na ₂ O	MgO	Al ₂ O ₃	SiO ₂	K ₂ O	CaO	FeO	MnO	Fe ₂ O ₃
1.37	0.99	12.13	65.95	1.95	3.63	0.07	0.02	1.22

Element Mass%		Amount of atoms %	Compound %	Formula		
Na	3.09	2.78	4.17	Na ₂ O		
Mg	2.03	1.72	3.37	MgO		
Al	7.61	5.82	14.38	Al ₂ O ₃		
Si	33.41	24.55	71.48	SiO ₂		
K	2.39	1.26	2.88	K ₂ O		
Са	0.65	0.34	0.91	CaO		
Fe	2.18	0.81	2.81	FeO		
0	48.63	62.72				
Sum	100					

Table 2 The elements that contain in Zeolite.

Then, using with FTIR spectroscopy functional groups present in the powder form of hybrid nanostructure identified. As a spectrum range interval from 4000 to 400 cm-1 at room temperature is taken. Then as a next stage, SEM analysis of the nanoparticle prepared by scanning electron microscopy (SEM) was taken on the SEM JEOL JSM-7600F Field Emission at 15KV accelerator voltage.



Figure 1. View of SEM analysis of clinoptilolite

After the experiment, the amount of CI ions was determined by titration. To determine how graphene oxide which obtained from the reaction affects the amount of CI- ions in water treatment, still water was filtered with graphene oxide and the amount of CI- ions was analyzed. According to the results obtained, the content of CI- ions in the water passing through the filter of graphene oxide was reduced by ~ 20%, and by 10% when using clinoptilolite.

STUDY OF COMPOSITE PROPERTIES ON THE BASIS OF FILLED HIGH DENSITY POLYETHYLENE

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The main modern global trend in the development of any type of product is the creation on its basis of a wide range of models, types, brands, modifications that ensure the effective development of a rapidly growing modern economy, expand the scope of products, and increase the volume of its release. This trend is fully characteristic of modern, especially thermoplastic polymer materials. The development of modern technology requires more and more new materials with properties established in advance, but the creation and development of the production of new polymers does not occur at all. That is why, the modification of known polymers, the development of polymer composite materials filled with functional additives, or mixed compositions, is currently one of the main directions in the creation of polymers and composites with predictable properties.

The purpose of our work is to develop composite materials based on filled low density polyethylene. The followings were used as fillers:

- graphene oxide an additive obtained by the "Hummers" method with additional oxidation and obtaining a variety of hydroxyl, carboxyl groups using hydrogen peroxide;
- red mud the residual of the processing of alunite of "Azeraluminium" Ganja plant, containing metal oxides, such as SiO₂, Al₂O₃, Fe₂O₃, K₂O, Na₂O and etc.

Taking into account the properties and composition of the fillers used, it is planned to obtain composites with high impact resistance, less brittleness, etc.

To prevent the degradation of polymer during processing at high temperatures, a polymer stabilizer with thermal stability was added into the composite before testing.

The following composites were prepared:

- 1. polyethylene + stabilizer + graphene oxide
- 2. polyethylene + stabilizer + red mud.

All components used are in a dispersed state. The filler was added into the polymer composition in an amount of $1 \div 5$ pts. wt. The pre-weighed components of the polymer composition - powdered polyethylene and a stabilizer, as well as a dispersed filler in a calculated amount are subjected to mechanical mixing for 5-10 minutes on a laboratory stirrer-mixer. Then, the obtained mechanical mixture is directed to the extruder for mechanochemical modification. The modification process was carried out at a temperature of 190-200°C for 3-5 minutes. After extrusion, the composition obtained is granulated.

To compare the properties of the original polyethylene and the modified composite based on polyethylene, the viscosity and melt flow rate (melt index) of the above-mentioned samples were determined on a capillary viscometer.

Based on the results of the studies carried out, we can say that with the addition of a dispersed filler into the polymer composition, the viscosity of the obtained compositions increases. As the amount of additive increases, the melt flow rate of modified mixtures decreases.

SYNTHESIS BASED ON A DERIVATIVE OF INDAZOLES WITH PHENACYLBROMIDE

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The reaction of functionalization of 4-aryl-4,5,6,7-tetra-hydro-2H-indazole derivatives of diacetyl substituted hydroxycyclohexanones with phenacyl bromide in boiling acetone in the presence of K2CO3 was investigated. The yield of the reaction product 2- (5-acetyl-6-hydroxy-4-R-3,6-dimethyl-4,5,6,7-tetrahydro-1H-indazole-1-yl)-1phenylethan-1-one makes 67-75%. X-ray structural analysis of a single crystal of 1- [6-hydroxy-4-(4-methoxyphenyl)-3,6-dimethyl-4,5,6,7-tetrahydro-2H-indazol-5-yl] ethanone, reveals the pyrrole and pyridine nitrogen atoms of the heterocycle, and alkylation with phenacyl bromide proceeds through more basic pyridine nitrogen.



Figure 1. Molecular structure of 1- [6-hydroxy-4- (4-methoxyphenyl) -3,6-dimethyl-4,5,6,7-tetrahydro-2H-indazol-5-yl] ethenone

The IR spectra of the compounds show absorption bands of stretching vibrations of the C = N group in the region of 1640-1625 cm⁻¹, carbonyl groups (C = O) of the acetyl substituent and aromatic ketone at 1702-1676 cm⁻¹, hydroxyl groups at 3390-3410 cm⁻ one. The absorption band of stretching vibrations of the secondary amine group (NH) is absent in the spectra of the compounds. According to the results of 1H NMR spectra of the compounds, the low-field hydrogen singlet of the NH group is also absent. Methyl proton signals were determined to appear as singlets at 1.22, 1.39, and 1.99 ppm. In the 13C NMR spectra of compounds, carbon signals confirming the introduction of a phenacyl group into the heterocycle are easily detected from a comparison of the 13C spectra of the starting compounds: signals with a chemical shift of 55.32 ppm. corresponds to the carbon of the CH2 group, 194 ppm. carbon C = O ketone groups. The reaction of phenacyl bromide with 3,6-dihydroxy-6-methyl-4-phenyl-4,5,6,7-tetrahydro-1H-indazole-5-carboxylate in boiling acetone and in the presence of K2CO3 leads to the O-alkylation product - ethyl 6-hydroxy-6-methyl-3-(2-oxo-2-phenylethoxy)-4-phenyl-4,5,6,7-tetrahydro-1H-indazole-5-carboxylate in boiling acetone and in the presence of K2CO3 leads to the negative charge is more dispersed on the oxygen atom, as on a more electro-negative element. On the other hand, acetone, being a polar aprotic solvent, favors the separation of the O⁻ // K + ion pair, thereby promoting O-alkylation.

EFFECT OF INORGANIC SALTS ON THE SOLUBILITY OF AMINO ACIDS

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INTRODUCTION

Proteins are complex molecules, and the direct study of their properties, such as solubility in aqueous salt solutions, has been proven to be quite complex from multiple points of view. Since solubility is essential to separate and purify proteins, using amino acids (AAs) or peptides as model compounds is a possibility to overcome this problem^{1,2}. As aqueous electrolyte solutions are the natural environments of many biomolecules, the study of the influence of ions on solubility is also important to improve the understanding of the behaviour of biomolecules in this environment.

DESCRIPTION OF THE WORK

The solubility data of amino acids in aqueous electrolyte solutions with molalities from 0 to 2 molal have been determined at 298.2 K. The studied AAs were L-aspartic acid (L-Asp), L-phenylalanine (L-Phe), L- leucine (L-Leu), and glycine (Gly). These AAs were chosen because they have functional groups with different polarities: L-Asp has a second negatively charged hydrophilic carboxyl side chain, Gly and Leu have nonpolar, hydrophobic groups, and L-Phe has a nonpolar, hydrophobic aromatic side chain. The salts consisted of the following ions: Na⁺, K⁺, and NH₄⁺ cations, and Cl⁻ and NO₃⁻ anions. The solubility of AAs was obtained through the isothermal shake-flask method combined with quantitative analysis by gravimetry. The solutions were stirred for 30 h and left to rest for at least 12 h. After each solubility measurement the pHs of solutions were also monitored.

RESULTS AND DISCUSSION

The obtained results show how the functional groups' presence affects the solubility of AAs. AAs with polar groups (L-Asp) present salting-in effect in all aqueous salt solutions in the whole molality range. The solubility of AAs with nonpolar groups (Gly, L-Leu, and L-Phe) increases slightly in the presence of salts, but the salting-out effect appears for higher molalities. In general, the salts with the nitrate anion induced a solubility increase higher than those with the chloride anion. This can be explained by the fact that the nitrate anion can interact more strongly3 with the apolar moiety of the AAs and increase their solubility. The relative solubilities of AAs with larger apolar functional groups were higher in aqueous solutions of salts with ammonium cation, while the relative solubility of L-asp was higher in solutions with potassium cation. Molecular dynamic simulations showed similar, but weak interactions, between all the studied cations and the carboxyl group of isoleucine (IIe), which also has an apolar moiety, but the binding of NH₄⁺ with the apolar moieties was somewhat more important⁴. The solubility results of L-asp in aqueous NaCl solution and Gly in all studied aqueous salt solutions were compared with the results from the literature. No data were found for L-Phe and L-Leu in aqueous salt solutions studied in this work. The pH monitoring showed that all AAs are in zwitterion forms in the aqueous solutions.

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SYNTHESIS BASED ON 5-METHYLCYCLOHEXANONE DERIVATIVE WITH PHENYLHYDRAZINE

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Macroheterocyclic compounds are good synthons for the synthesis of new substances with the antimicrobial properties and best physicochemical characteristics. Currently, the synthesis of new organic compounds that can be used as anticancerogenic substances, such a series that serve to delay the replication of cancer cells, is one of the most pressing problems of modern chemistry. When considering new methods for the synthesis of macro-heterocyclic compounds based on the derivatives of cyclhexanalones, we have studied the reaction of synthesis based on benzaldehyde or 4-methylbenzaldehyde and acetylacetone with substances containing diamine fragments.

We carried out the reaction of 3-phenyl-2,4-diacetyl-5-hydroxy-5-methylcyclohexanone with phenylhydrazine in ethanol in the presence of a catalytic amount of concentrated hydrochloric acid. According to the results of the reaction, after chromatography on a column filled with an adsorbent silica gel, we isolated two products.

To a mixture of 0.576 g (0.002 mol) of our synthon with a calculated amount of 0.216 g (0.002 mmol) of phenylhydrazine in 20 ml of ethanol was added 1 drop of concentrated hydrochloric acid, this reaction was carried out at 50-55°C. Monitoring the progress of the reaction is carried out by TLC eluent - ethyl acetate-hexane 1:1. After the formation of the substance, the solvent was evaporated, that is, the resulting residue was chromatographed on a column filled with aluminum oxide, using ethyl acetate – hexane 1:1 as the eluent. At the end of the reaction, two fractions were isolated.

GLYCEROL VALORISATION TOWARDS BIOFUEL ADDITIVITIES: THERMODYNAMIC STUDIES OF GLYCEROL ETHERS

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Most processes in the chemical industry use the traditional organic solvents. Although there are apparent advantages in the use of these kinds of solvents, such as availability and low price, there are some important drawbacks such as their volatility, flammability, and toxicity. That is why, the development of inexpensive, harmless and environmentally friendly alternative solvents is of great importance. The glycerol ethers fully meet the renewable green solvent requirements and have attracted a great deal of attention in various applications. Glycerol ethers in particular have proven to be promising candidates for solvent substitution, since their physicochemical properties can be modulated by the number, size, and type of their alkyl groups, which among other things leads to a wide range of polarities. Experimental properties of glycerol ethers are practically absent in the literature. Knowledge of reliable thermodynamic data is essential for the design and development of new technologies.

Glycerol and its derivatives provide a versatile substrate for the design and synthesis of new, bio-derived compounds that can have uses in key contemporary applications such as CO₂ capture, plastics recycling, and green chemistry in general. Upon etherification of one or more alcohols the glycerol skeleton, the thermophysical properties of the resultant substances change dramatically compared to glycerol. Most notably, the viscosity of glycerol-derived diethers and triethers is reduced by 2-3 orders of magnitude, however, this also corresponds to increased volatility. Determining properties of these new compounds is a key consideration for engineering process design. Here, for the first time we report on the vapor pressures, heat capacities, and enthalpies of vaporization of symmetric 1,3-diethers of glycerol and provide a group additivity model for estimating the enthalpies of vaporization. The properties of these glycerol-derived solvents are compared to other compounds with similar structures.

DETERMINING THE OPTIMUM OPERATING PARAMETERS OF A CASCADE REFRIGERA-TION SYSTEM UTILIZING THE R227ea (1,1,1, 2, 3,3,3- heptafluoropropane) REFRIGERANT

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Successive two-stage refrigeration systems are widely utilized, especially for low-temperature cooling applications. One of the important steps to be taken for the more efficient operation of such systems is the selection of the refrigerant to be used in the system. Because achieving the highest COP value in refrigeration cycle depends particularly on the selection of refrigerant and detecting the optimum operating parameters. R227ea (1,1,1,2,3,3,3- heptafluoropropane) can be used as alternative refrigerant for CFCs and HCFCs because of its zero ODP, acceptable GWP, high COP, low discharging pressure less than 2.5 MPa. However, their applications are limited because of its flammability. In this study, as an example, a two-stage refrigeration cycle model using R227ea refrigerant was developed and the optimal operating conditions of the system were determined. For this purpose, a simulation model was improved by using Java language. In this model, stochastic (statistical) optimization methods were used to prevent possible errors. In addition, a separate simulation model was developed in Java language for determining the thermodynamic properties of all phases of the refrigerant. In the mathematical model improved for the determination of thermodynamic properties, the properties for the liquid and superheated vapor zones were figured out using the Helmholtz real gas state equation. The saturation properties of the refrigerants were also detected using the cubic spline polynomial equations. It was observed that the results obtained from this simulation study are significantly compatible with the actual cooling cycle and the model developed in this study will provide significant advantages, especially in the system design and analysis stage in industrial cooling applications.

KEYWORDS: Refrigerants, thermodynamic properties, refrigeration cycles, R227ea.

VISCOMETRIC STUDIES OF BINARY AND TERNARY LIQUID MIXTURES

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Viscometric properties are very important to study the nature and extent of intermolecular interactions. The presence of COVID-19 in our midst has brought experimental research to a standstill and the looming global threat of the third wave has thrown the entire world in a turmoil. All across the world, research labs are in a complete shutdown mode. Keeping that in mind, an attempt has been made to predict the viscometric properties of binary and ternary liquid mixtures using 10 different approaches which includes some well-established and some recently developed approaches. These predictive approaches encompass some approaches which have been used for decades, viz., Bingham, Kendall-Munroe, Frenkel, Hind & Ubbelohde, Eyring, Sutherland Wassiljewa and some recent models like Modified Frenkel, Linear and logarithmic approaches and the recently developed Dey-Biswas and tested over a range of temperature. Average Absolute Percentage Deviations (AAPD) has been used as the criterion for determining the efficacy of their predictive capability.

More than 200 plus binary mixtures and 25 ternary mixtures comprising of components of varying size, shape, orientation and constitution have been included in the present investigation. The investigation also includes systems comprising of lonic Liquids as one of the components, as their behaviour is very different from organic liquid mixtures and the comparative study will shed some light on the predictive efficacy of the chosen approaches. The findings shows that the recently developed the Dey-Biswas approach exhibits superior predictive capability than all the other approaches for binary as well as ternary liquid mixtures.

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CALCULATION OF EQUILIBRIUM COMPOSITION OF COMPLEX THERMODYNAMIC SYSTEMS USING JULIA LANGUAGE AND IPOPT LIBRARY

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The problem of calculating the equilibrium composition of multicomponent heterogeneous thermodynamic systems is rather old. The first algorithms and programs for calculating the equilibrium composition appeared in the late forties and early fifties of the 20th century. The development of such programs has made it possible to significantly reduce the costly, complex and hazardous experimental studies of rocket fuel compositions. The first algorithms for calculating the equilibrium composition used the method of equilibrium constants, and it was necessary to solve a system of nonlinear equations. But when solving a system of nonlinear equations, several solutions are often possible and it is not always clear, which one is true, so the method of equilibrium constants is not widely used. Later appeared the algorithms and programs for calculating the chemical equilibrium, which were based on the method of minimizing the Gibbs energy. Now the methods of minimizing the Gibbs energy or Helmholtz energy are much more often used to perform thermodynamic calculations.

The present study is dedicated to analysis of the possibility of using the lpopt optimization package for the calculation of the phase and equilibrium compositions of a multi-component heterogeneous thermodynamic system. Two functions are presented for calculating the equilibrium composition and properties of complex thermodynamic systems, written in the Julia programming language. These functions were integrated with the IVTANTHERMO database on the thermodynamic properties of individual substances and used to carry out the test calculations. As our experience shows, the Ipopt package allows one to determine the phase and equilibrium composition of simple and complex thermodynamic systems with a fairly high speed. Using the JuMP modeling language significantly simplifies the preparation of source data for the lpopt package, so the functions for the calculation of chemical composition are very compact. It is shown how the loopt package can be used in the case when the temperature of the thermodynamic system is unknown. The approach proposed in this work is applicable both for analyzing the equilibrium of individual chemical reactions and for calculating the equilibrium composition of complex chemically reacting systems. The compactness of the functions presented allows one to easily embed them into more complex applications, use it in combination with more complex models (real gas, nonideal solutions, constrained equilibrium), modify them if necessary. It should be noted that the versatility of the JuMP modeling language makes it possible to replace the lpopt package with another one without significant modification of the program text.

SOLID LIQUID EQUILIBRIA OF BINARY SYSTEMS: EXPERIMENTAL DATA AND MODELIZATION

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Solid–liquid equilibria (SLE) of the *n*-eicosane with biphenyl, dibenzofuran, and indole covering the whole composition range were measured by differential scanning calorimetry (DSC) technique in a temperature range 309-356 K. The binary systems studied are completely miscible in the liquid state but non miscible in the solid state, and it was found that all the systems exhibit simple eutectic points. The experimental data were predicted by ideal solution model; by two versions of the modified UNIFAC model, Lyngby and Dortmund versions. Errors in the prediction of activity coefficients are slightly high but predicted melting temperatures are very accurate. The best description is obtained with Modified UNIFAC (Lyngby) model, which leads to the lowest deviations in melting temperatures and activity coefficients. Systems including *n*-eicosane are characterized by positive deviations from the Raoult's law, which are stronger in indole solutions.





KEYWORDS: DSC, Solid-liquid equilibria, Activity coefficients, *n*-eicosane, UNIFAC.

MULTIPHYSICAL MODELLING OF A FERROFLUID BASED SINGLE-PHASE NATURAL CIRCULATION MINI LOOP

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Ferrofluids are suspensions of nano-sized ferromagnetic particles in a non-magnetic conventional heat transfer fluid. They have great research of interest to be used as heat transfer media in industrial applications, due to their temperature dependent magnetization property and magnetic field dependent thermophysical, acoustical, optical and electrical properties. In this study, the effect of using water based Fe₃O₄ ferrofluid on the performance of a single-phase natural circulation mini loop, as passive components of heat transfer systems, has been investigated numerically. The numerical model was developed by coupling three different physics in the COMSOL Multiphysics: magnetic field (without currents), heat transfer and fluid flow (laminar flow). The influence of the magnetic field was introduced as a magnetic volume force and a magnetocaloric effect to the momentum and energy equations, respectively. Herein, the magnetic volume force is caused by the generated magnetic field gradient in the fluidic domain, where the magnetocaloric effect is a result of both generated magnetic field gradient and the magnetization change due to the temperature. To evaluate the performance of the ferrofluid based single-phase natural circulation mini loop under the influence of the magnetic field, the maximum temperature (T_{max}), the temperature difference between heater inlet and outlet (ΔT_{heater}), and the effectiveness (ϵ) parameters were considered. Moreover, the velocity and the temperature distributions at the critical cross-sections of the geometry were investigated.

MULTI-WALLED CARBON NANOTUBE-BASED NANOFLUIDS: FROM KNOWLEDGE TO INDUSTRIAL APPLICATION

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The development of technologies using renewable sources, such as solar panels, geothermal energy, and the need for high-efficiency cooling in the area of batteries in electric vehicles or the electronics industry, forces the search for more efficient types of heat transfer fluids. High requirements of specialty liquids are met by nanofluids composed of nanoparticles dispersed in base liquids.

The formation of stable dispersions of nanoparticles in base liquids such as glycol or water is the first step in the commercialization of nanofluids. However, industrial heat transfer fluids contain specialized additives such as corrosion inhibitors, antifoams and biocides, which significantly hinder the formation of stable systems. An additional challenge is to move the nanofluid manufacturing process from laboratory scale to a production process.

The nanofluids under study are composed of commercially available multi-walled carbon nanotubes MWCNTs and water-glycol base with additives (corrosion inhibitors, antifoam agent). The polivinylpyrrolidone as a nanotubes stabilizer was used. The usage of nonpetroleum origin glycols provides to achieve bio-based, sustainable products with highest performance and quality. The dispersion were prepared by two-step procedure using sonication method.

In this work, a manufacturing process was designed to enable the production of nanofluids. Thermal conductivity, viscosity and stability at various temperatures of obtained nanofluids are presented.

CALORIMETRIC STUDIES OF GAS HYDRATE FORMATION AND DISSOCIATION FOR MIXTURES OF METHANE, ETHANE, PROPANE AND ISOBUTANE FOR THE LOW CONCENTRATION OF C2+ COMPONENTS

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Adiabatic calorimetry is used for the thorough studies of gas hydrate formation and dissociation of mixtures of methane, ethane, propane and isobutane for the low concentration of C_{2+} components. These mixtures are similar (concerning to the composition of hydrate forming components) to the natural gas of some gas-condensate fields of Siberia in Russia. Original adiabatic calorimetry setup is described in detail. Heat capacity, internal energy, pressure, and temperature derivative of pressure at constant volume for these systems have been measured in the hydrate's forming range. Based on the experimental data of heat capacity, internal energy, pressure, and temperature derivative of pressure at constant volume the phase diagrams for gas hydrates have been plotted. Phase transitions are localized by the finite discontinuities in temperature derivatives of the thermodynamic potentials.

Our investigations show that phase behavior of hydrocarbon mixtures of methane, ethane, propane and isobutane for the low concentration of C₂₊ components at the thermobaric conditions of hydrate formation has got the complex nature. These hydrocarbon mixtures have formed double and mixed hydrates. The each size cage of double hydrates is primarily occupied by a different type of molecule. The same size cages of mixed hydrates are occupied by different types of molecules, with the restriction of at most one molecule per cage. The thermobaric domain of gas hydrate occurrence is not uniform, but it is divided into the set of ranges with the different crystal structures. Phase transitions from one structure to another are accompanied by the structural phase transitions. Heat of hydrate fusion and ratios of different crystal structures have been defined. An extensive thermobaric domain of the state of metastability of the water - hydrocarbons systems has been studied. Research of sufficient stable region of the metastable state of the intermediate water - hydrocarbons system in the productive reservoir (at the bottom-hole zone) makes it possible to more reliably evaluate the risks and probability of hydrate formation at the thermobaric conditions of these hydrates occurrence. Using experimental data some speculations on hydrate formation at bottom-hole zone are discussed.

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CHALLENGING SEASONAL SEA-WATER PARAMETER FLUCTUATION FOR S.W.R.O (SEAWATER REVERSE OSMOSIS) DESALINATION PLANTS: A GLOBAL PARAMETRIC SURVEY FOR LOCATING THE CRITICAL AREAS – BASED ON ANALYSIS OF COPERNICUS MULTI-OBSERVATION OCEAN DATA 1993-2021

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Many countries depend on seawater desalination for both potable and agricultural uses and after four decades of successful use of such plants, it turned to one of the most reliable solutions to water scarcity worldwide. As claimed for decades, seawater desalination supposed to be climate-independent source of water, which helped many countries secure their water supplies against the climate change, growing population and drought.

The membrane-based desalination techniques has the biggest share in large-scale sea-water desalination plants and RO (reverse osmosis) is the oldest and the most mature technology which is almost reaching it's theoretical limits. Off course avoiding over-and under-design and fine-tuning the economic and exergy requirements is the main priorities in such designs.

In the current work, we have started with briefly demonstrating the effect of important seawater parameters on SWRO desalination efficiency and then went into details of seawater salinity change as the main parameter of interest to have a quantitative view of salinity change effect on energy performance of such plants. On the other hand, based on the sea surface salinity and water density values from Copernicus multi-observation ocean data of 1993 to 2021 across the global ocean we made a seasonal salinity change analysis and high-lighted the critical areas - around the world - with the highest salinity changes. It is shown most of such areas are Atlantic and Car-ibbean islands which are already in need of seawater desalination plants. This simply high-lights the need for more detailed researches on novel designs and multi-variable optimization methods to fine-tune the wide-range of salinity changes.

ISOBARIC HEAT CAPACITY OF IONANOFLUIDS WITH FUNCTIONALIZED AND NON-FUNCTIONALIZED MULTI- WALLED CARBON NANOTUBES

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The ionanofluids (INFs) can exhibit excellent thermal conductivity due to addition of multi-walled carbon nanotubes (MWCNTs) [1]. Whereas effect of MWCNTs on isobaric heat capacity (C_p) still remains not fully explored as can be seen in contradictory results shown in the literature [2,3]. This work is aimed to further study of the isobaric heat capacity of INFs. Three different ionic liquids were investigated, 1-ethyl-3-methylimidazolium thiocynate [EMIm][SCN], 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [BMPyr] [NTf₂], 1-proyl-1methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [PMPyr][NTf₂] and nine INFs based on those liquids. Long MWCNTs and functionalized MWCTNs with carboxylic group (MWCNTs-COOH), carbon chain (MWCNTs-C₁₈) and poliethylene glicol (MWCNTs-PEG) were used for two step preparation of INFs.

This research shows that for [EMIm][SCN] + 0.5 wt% MWCNTs-COOH and [EMIm][SCN] + 1 wt% MWCNTs-PEG the isobaric heat capacity increases by 3.1% and 2.6% at 323 K, respectively. The addition of nonfunctionalized MWCNTs resulted in increase of isobaric heat capacity of INFs by 2.6% at 323K for [PMPyr][NTf₂] + 1 wt% MWCNTs. While, the C_{ρ} of [EMIm][SCN] + 2.5 wt% MWCNTs-C₁₈, like [EMIm][SCN]based INFs with non-functionalized MWCNTs, remains unchanged. Hence, it seems that addition of MWCNTs functionalized by polar groups may be a good way to obtain the real increase in the isobaric heat capacity.

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PERFECT GAS EQUATION OF STATES FOR THERMODYNAMIC PROPERTIES OF PURE GASES AND GAS MIXTURES AND THERMOPHYSICAL PROPERTIES OF PERFECT GASES AND GAS MIXTURES

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The simplest thermodynamic description of gases are ideal gas Equation of State. Ideal gas definition is given us a limited description of thermodynamic behavior of gases. It is serror levels increases in low temperatures, high pressures and around critical point. Yet, it is one of the most used equation of state due to simplicity. For perfect gases properties such as enthapy and entropy is reduced to be only function of temperature. These simplify some complex processes such as chemical equilibrium calculations and gas mixture calculations. For gas mixture, it has a further simplification of ignoring interaction effects between different molecules. The ideal gas equation of state has the form

$$P = \frac{NRT}{v}$$

In this equation *P* is pressure, *N* is moles of species, *R* is universal gas constant, *T* is temperature and v is specifiv volume. In order to calculate thermodynamic properties such as enthalpy, internal energy, entropy ideal gas equation alone is not sufficient additional information is rquaired and this information is usually given in the form of C_p , specific heat. Specific heat data for gases can be obtain from several resources such as National Institute of standards and technology of U.S: Department of Commerce (NIST) databases. They are known as JANAF Tables. Another important sources of C_p data can be found in Ihsan Barin Thermochemical Data of Pure Substances. Some sources offers data in the form of curve fitting values (mostly in polynomial form). Most noted of this data form is National Air and Space Administration (NASA) data which is developed originially for the moon mission of 60's.

Several different way of utilising C_p data is possible. As curve fitting models Partial continious curve fitting is one of the accuretae way of modelling curve fitting

$$C_{pi} = A_i + 10^{-3}B_iT + 10^5 \frac{C_i}{T^2} + 10^{-6}D_iT^2, \quad T_{Li} \le T \le T_{Hi}$$

Another model utilizes cubic spline method to accurately define Cp values

$$C_{pk}(T) = a_k (T - T_k)^3 + b_k (T - T_k)^2 + c_k (T - T_k)^3 + C_{pk}(T_k), \quad 1 \le k \le n$$

In NASA database and other sources CP values are given directly as polynomial curve fitting as one or more than one temperatre zone(partial difference form) Avantages of this data source is having a rich collection of data availibility up to 6000 K.

Several perfect gas equation of state developed by utilising these big array of sources. Furthermore themophysical properties such as viscosity and thermal conductivity data of perfect gases ahould be defined in order to utilised these PG EoS' in heat transfer calculations. Two approaches used for this purposes: If data is available, it is added into the program as curve fitting models, when data is not available, general equations for estimation of thermophysical properties are used.

In order to calculate ideal gas mixtures, ideal gas mixing rules applied. to calculate thermophysical properties of ideal gas mixtures wilke equation is used. The codes are developed in java programming language. The program code are given to interested researchers as free access in <u>www.turhancoban.com</u> adress.

KEYWORDS: Thermodynamic properties of gases, perfect gas EoS, thermophysical properties of perfect gases.

THERMAL PROPERTIES OD 1-ALKYL-3-METHYLIMIDAZOLIUM BIS(TRIFLUOROMETHYLSULPHONYL)IMIDE-BASED NANOFLUIDS

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Carbon based ionanofluids (INFs) show significantly better heat transfer properties in comparison to base ionic liquids. Sometimes even synergic effect can be observed and results exceed expectations.

We examined the effect of alkyl chain length in cation of the ionic liquid on the thermal conductivity and density of INFs. We prepared three series of INFs in concentrations from 0.25wt% to 2wt% of multi walled carbon nanotubes (MWCNTs, average diameter 60-80 nm, average length 770µm) based on 1-ethyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide [EMIm][NTf₂], 1-ethyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide [BMIm][NTf₂], 1-hexyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide [IMIm][NTf₂].

Unremarkable thermal conductivity enhancement of 170%, 174% and 182% with addition of 2wt% of MWCNTs to respectively [EMIm][NTF₂], [BMIm][NTf₂] and [HMIm][NTf₂] has been observed. The longer the chain length in cation of ionic liquid the higher the increase in thermal of thermal conductivity in nanofluids. Also the conductivity increase shows non-linear dependence on concentration of MWCNT in nanofluid.

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ABOUT ROCKS EFFECTIVE THERMAL CONDUCTIVITY PT- DEPENDENCES

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We presents the results of experimental measurements of the effective thermal conductivity of sandstone rock samples for the temperature range of 273-523 K under pressure conditions of 0.1-400 MPa. [1-3] Based on the analysis of literature data and the results of experimental measurements, we have shown that the temperature dependence of disordered media does not obey the laws of Eucken and Debye. A mathematical model is proposed that describes the power-law nature of the dependence of the thermal conductivity of disordered media on temperature and pressure.

Applying the power law to both the variable (T) and fixed (T_0) temperatures, in describing the temperature-baric dependence of thermal conductivity, we went over to dimensionless quantities, having obtained the following equation:

$$\lambda(T, P) = \lambda(T_0, 0) \cdot \left(1 + \delta_{T_0}(P)\right) \cdot \left(\frac{T}{T_0}\right)^{n_0 \cdot (1 - \nu(P))}$$

This representation makes it possible to distinguish only two reference quantities $n_0 = n(0)$ and $\lambda(T_0,0)$, and two dimensionless pressure functions $\nu(P)$ and $\delta_{T_0}(P)$. Both quantities are usually well described by two-parameter expressions, which are discussed in the report. Thus, to obtain a description of the temperature-pressure dependence of the thermal conductivity of most of the investigated composite materials, in particular, such rocks as granites, sandstones, etc. The relationship between value and sign of $n = n_0 \cdot (1 - \nu(P))$ and structural ordering is discussed.

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STUDY OF THE ANTIMICROBIAL PROPERTIES OF 1- (6-HYDROXY-3,6-DIMETHYL-2,4-DIPHENYL-4,5,6,7-TETRAHYDRO-2H-INDAZOL-5-YL) ETHAN-1-ONE

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The synthesis of new macroheterocyclic compounds is currently relevant because they can reveal pronounced antimicrobial properties and a new class of drugs can be created on their basis. Among them the cyclohexanalones, can be synthesized by the reaction of diacetyl substituted1,3-dioxo compounds with diamines. One of the methods for the preparation of N-phenylpyrazoles, which have a wide spectrum of biological activity, is the reaction of phenylhydrazine with symmetrical 1,3-dioxo compounds.

The reaction of 2,4-diacetyl-3-phenyl-5-hydroxy-5-methylcyclohexanone as a compound containing an asymmetric 1,3-dioxo moiety with phenylhydrazine was carried out to investigate the direction of the attack of the nitrogen nucleophilic centers of phenylhydrazine with the carbonyl groups of the cyclohexane ring. The reaction was carried out by heating in ethanol in an equimolecular ratio of reagents. Separation by column chromatography isolated two products: 1- (6-hydroxy-3,6-dimethyl-2,4-diphenyl-4,5,6,7-tetrahydro-2H-indazol-5-yl) ethan-1-one and 1- (2-hydroxy-2-methyl-6-phenyl-4- (2-phenylhydrazono) -5- (1- (2-phenylhydrazono) ethyl) -cyclohexyl) ethan-1-one in 52% and 15 % respectively:



Figure 1. Molecular structure of 1- (6-hydroxy-3,6-dimethyl-2,4-diphenyl-4,5,6,7-tetrahydro-2H-indazol-5-yl) ethan-1-one

When studying the antimicrobial properties, rivanol and furacselin drugs were taken for comparison, and according to the results it was found that 1- (6-hydroxy-3,6-dimethyl-2,4-diphenyl-4,5,6,7-tetrahydro -2H-indazol-5-yl) ethan-1-one has the best antimicrobial properties compared to model medicines. The structure of the synthesized compounds was studied by IR NMR spectroscopy, and X-ray structural analysis was used to determine all characteristics, including torsion angles and conformations. As can be seen from fig.1, intermolecular hydrogen bonds were also determined.

ENERGY STORAGE BASED ON THE ADSORPTION PROCESS

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The most of world's energy demand is still produced from fossil fuels which in its final form causes significant influencing of environment. In addition, the energy demand will still increase in future extensively. Thus the present focus is on the use of renewable energy sources and modern technologies applied in energy extraction and recycling. The presented work concerns thermal energy storage systems which correspond with mentioned environmental and energy demand requirements. These systems are applied on high efficient technologies for application in heating and cooling systems for buildings. Our research is then pointed at their working cycles (charging and discharging cycles) for which was designed a testing storage system at our university.

The storage system was designed to conduct the testing with a silica gel absorbent material in loose globular form. The storage system consists of insulated sorption tube, mixing chamber, heat gun, atomizer and its water supply system connected to pump and pipes connecting all components. Absorbent is inserted in sorption tube. Thermocouples, sensors of relative humidity and flow velocity are placed across the storage system. The adsorption phase works with heat gun and atomizer in process. The moist air flows through sorption tube. Heat is then released when adsorption occurs since the process is exothermic and stored as sensible heat. During inverse phase the storage system works without atomizer and working fluid is heated to higher temperature. The desorption is causing a release of moisture from the absorbent. Based on this system is tested main goal of our research – degradation in the storage density of the absorbent for certain working period and for repeated cycles.

The design equipment will be used for testing of the common applied substance for the energy storage by the adsorption process. The main advantageous will be the fully automatic control system which allows preforming many adsorption-desorption cycles under various working conditions. In the previous publications the test device was successfully design and used for silica gel testing as was mentioned above. The new concept is now under construction and it is scheduled to be in the service soon. Using new testing concept, the other materials e.g. zeolite etc. can be used.

KEYWORDS: energy storage, storage system, silica gel, adsorption, desorption

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GRAPHENE OXIDE-DIHYDROPYRIMIDINE BASED SUPRAMOLECULAR ENSEMBLES AS AN EFFECTIVE ANTIBACTERIAL AGENT

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The Biginelli reaction, which is a classic example of one-pot multicomponent reactions, is a powerful and versatile tool for designing and constructing dihydropyrimidines, a unique class of heterocyclic molecules having two nitrogen atoms in the cycle. Despite using simple starting components such as aldehyde, urea derivative, and methylene active molecule, the reaction's effectiveness is due to the tremendous complexity and diversity of the products. The numerous research publications and reviews published on this issue thus far demonstrate the scientific community's great interest in the Biginelli reaction, which has led to dihydropyrimidines becoming well-known in medicine. Dihydropyrimidines have a wide range of biological activities, which explains their repute. According to numerous studies, these chemicals have anti-leishmanial, anticancer, antiviral, antifungal, antiproliferative, antibacterial, anti-inflammatory, antihypertensive, antiepileptic, anti-HIV, antidiabetic, anti-malarial, mPGES-1 inhibitors, antitubercular and other activities.

On the other hand, graphene oxide is a promising chemical that is gaining in popularity every day (GO). It is a multilayer single-atomic substance with oxygen-containing groups created by a vigorous oxidation of inexpensive and plentiful graphite. These functionalities provide easy dispersibility of GO in water and other organic solvents, as well as in various matrixes. The characteristics of GO can be significantly altered by functionalizing it. Chemically modified graphenes could be used in a variety of applications, which underlines ist importance.

Considering all mentioned, we report of the synthesis of a new hybrid material on the basis of nanolayers of GO and dihydropyrimidines. Dihydropyrimidines, which were obtained by the condensation of 2,4,6-trimethoxybenzaldehyde with urea and acetylacetone/methyl acetoacetate, were used as a substrate. The structure of the obtained dihydropyrimidines was confirmed by ¹H and ¹³C NMR and mass spectroscopy methods as well as elemental analysis. Hirshfeld surface and contact enrichment ratios were obtained with MoProViewer. For the electrostatic energy calculation, the charge density parameters were transferred from the ELMAM2 database of multipolar atoms. The electrostatic energy was computed with the VMoPro module of MoPro software between pairs of atoms in close contact up to a cutoff of sum of van der Waals radii plus 0.5 Å. The average E_{elec} value was obtained by dividing the summation by the number of contacts. The structure and morphology of GO based ensembles were studied with TEM, XRD and FTIR methods.



Considering the biological activity of the graphene oxide based ensembles, obtained hybrids were analyzed against various gram-positive and gram-negative bacteria and promising results were obtained.

HEAT TRANSFER IN PARTIALLY-MISCIBLE BINARY MIXTURES UNDER HIGH POWER HEAT RELEASE: EXPERIMENT AND MODELING

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The current technological trend is to increase the intensity of processes while reducing the size of devices down to mini- and micro-sizes. It contributes scientists' interest to theoretical and experimental study of heat transfer features in multiphase heat carriers, which can be potentially applied in micro heat exchangers. Partially-miscible binary mixtures having a limited (in a certain region of the temperature-concentration phase diagram) compatibility of components are one of these coolants [1]. When crossing the line of phase coexistence, such mixtures are separated into two liquid phases. The separation process occurs by either nucleation or spinodal decomposition.

Nucleation is a localized process and requires the energy barrier overcoming for formation of nuclei that later grow and coalesce. Spinodal decomposition, instead, is a delocalized process and it occurs simultaneously in the entire domain without the energy barrier overcoming: concentration fluctuations are amplified and lead to the separation of the initially single-phase binary solution into the two-phase region with different equilibrium concentrations. It is assumed that for low-viscous liquids, in which the diffusion coefficient is relatively small, the process of spinodal decomposition is accompanied by self-induced convection. Appearance of the convection mode leads to heat transfer enhancement.

Despite the fact that the kinetics of the phase separation process in partially-miscible mixtures has been studied for more than 60 years [2], today there are practically no works devoted to the heat transfer investigation in such mixtures in case of small characteristic heating times (1-180 ms), sizes (~10 µm) and high heat flux density (10-15 MW/m²). Such conditions make it possible to carry out experimental thermophysical studies in the region of not only fully stable thermodynamic states but also in the region of not fully stable or unstable states. The term "not fully stable" implies mixtures that are superheated for a short period of time with respect to the liquid-liquid equilibrium line. The term "unstable" is used for mixtures that are superheated with respect to the diffusional spinodal. For these purposes, the controlled pulse heating method of the platinum wire probe has been applied. The thickness of the platinum wire is 20 µm, the length is ~ 1 cm. The heating rate ~106 K/s. The initial state of mixture corresponds to the region of thermodynamic stability. This approach allows the heat release parameters to be directly controlled in the probe during the pulse, as well as allowing the response function to be recorded across the heating range. During the pulse heating the voltage drop across the probe and the voltage drop across standard resistor, converted to the current in the probe circuit, are recorded as functions of time. Registration of primary data is accompanied by calculations of the heat release power and the temperature of the probe - resistance thermometer as well as the heat flux density through the probe surface. The method is described in more detail in [3]. Pressure serves as a parameter. The water/polypropylene glycol-425 (PPG-425) mixture having lower critical solution temperature (hereinafter LCST) has been chosen as an object of study. The estimate of the LCST coordinates for this solution known is as follows: 328 K and 0.27 PPG-425 wt.fr. Water and PPG-425 are non-toxic, easily available substances that can be used in large quantities.

The specificity of the heat transfer pattern was detected in the composition range from 0.1 to 0.4 PPG volume fraction corresponding to the region of unstable states. The analysis of the probe temperature in time T(t) at a given heating power P(t) showed two characteristic features. Firstly, despite the relatively large value of heat flux density (~ 14 MW/m²), tendency to the formation of the temperature "plateau" was observed. We attribute this observation with the spinodal decomposition onset which is the most powerful and natural relaxation process in this region of the phase diagram. Secondly, going deeper into the region of unstable states, ordinary order in amplitude of response curves (with respect to step-by-step pressure increase) changes to the opposite: lower values

of the heat transfer intensity begin to correspond to higher pressure values. It can be explained by an increase in the LCST temperature with pressure accompanied by a narrowing of the spinodal-confined region [4].

In addition, in the report the theoretical description of the experimental results will be presented. In accordance with the developed model, the growth of separated phases domains in a temperature gradient field leads to the appearance of thermocapillary forces. For this reason, small domains start to move towards each other and engage intensive micro convection in heat transfer process. Also, within the framework of the model it was shown

that the growth rate of domains of separated phases is proportional to \sqrt{t} .

Thus, in this work, we have obtained unexpected results that complement the results of stationary experiments and can serve as a practical basis for the search of a new generation of coolants for processes involving powerful local heat generation.

KEYWORDS: non-stationary heating, high heat release, partially-miscible mixtures, spinodal decomposition, lower critical solution temperature, aqueous solution, thermocapillary forces

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THERMODYNAMIC SPEED OF SOUND MEASUREMENT OF XENON WITH THE PULSE-ECHO TECHNIQUE

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Because of its distinct and non-reactive character, xenon has numerous applications in medicine, nuclear magnetic resonance (NMR) spectroscopy, illumination and optics, as a solvent and spacecraft fuel [1,2]. Because the global demand of xenon is increasing rapidly, accurate thermodynamic data become more important to optimize its usage and supply. The speed of sound is a full-fledged thermodynamic property, when amplitude and frequency are not excessive. Due to its caloric and thermal nature, temperature and pressure dependent thermodynamic speed of sound data are essential for the development of Helmholtz energy equations of state. Moreover, the according measurements can be accomplished comparably rapidly and yield data with a high accuracy [4]. In the present work, xenon is sampled with the double path length pulse-echo technique to provide the speed of sound data, covering a temperature range from 217 K to 500 K with a pressure of up to 100 MPa. At a confidence level of 95% (k = 2), the data have an overall expanded uncertainty of up to 0.17% near the critical point and less than 0.1% in the liquid and supercritical regions. The results are in good agreement with the Helmholtz energy equation of state by Lemmon and Span with a maximum deviation of up to 1.1%. The present data are also used to optimize the parameters of the Lennard-Jones potential and its truncated and shifted form for xenon. This parameterisation leads to a convincingly better performance for the speed of sound calculation, but the representation of other properties, like the vapour-liquid two phase region, is significantly deteriorated.

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EFFICIENCY OF SOLAR ENERGY APPLICATION FOR STOPPING DEFORESTATION

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Ecoenergetic effectivness of solar energy potential of Azerbaijan have been worked out within several projects up today. Locally energy potentials in the regions with the forest especially on the mountanous zones weren't perfectly studied from ecoenergetic and ecoeconomical facets.

Though the thermal balance was established but this doesn't mean the energy potential. As the research object the Mountaionous Shirvan agroecological region was selected for estimation of local solar energy resource. As the modern way especially aerospace observation method was used in the research by using several satellite materials done by different international Space Agancies and companies such as; DeLorme, UNEP-WCMC, USGS, NASA (Landsat), ESA, METI, NRCAN, GEBCO, NOAA, IPC, MERRA 2 (NASA), SHARE (BMT) and weatherspark.com.

Accordingly solar energy potential of the agroecological region was estimated and mapped. Initially DEM (Digital Elevation Model) of the Mountainous Shirvan has been developed. There are 5 administrative region including Khizi, Ismayilli, Shamakhi, Agsu and Gobustan in this agroecological region. On this base the initial total solar energy potential map was worked out. In order to economize forest wood the local solar energy resource should be applied to stop deforestation. Because the total area of the agroecological region consists of 684 000 ha land area in the zone including 82 000 ha woodland area. This showing is about 12%, so that's less than the international standards many times. In this case the forest lines have to be certainly secured in time to escape the nature complex loss. Mainly heating causes the long term exploitation of the forest wood in the region. Using solar energy resources can solve the heating the lightening problem of the Mountainous Shirvan. There are 225 sunny days and cloudness is less in the region having open sky condition mostly because of the mountain-valley wind potential and often raining or smowing depending on the seasons.

Due to the relief plastic being 2713 m height and -3 minimum index the territory is divided into 3 (three) potential zones such as; high, middle and low ones. The high potential is observed on the highest mountainous region and the lowland territory of Gobustan due to the georaphical location.

Because of the compound relief structure of the agrarian region the gas pipeline building process is possible but difficult at the same time. After the burning the natural gas a lot of hazardous wastes include into the atmosphere. Much more forest complex is demanded to clean them out. To stop the deforestation, woodland safety is actual and permenant woodlanding deeds are needale at present. The woodland complex saves the atmosphere, the soil cover and matrix and regulates the mountainous river branches, springs and underground water sources at the same time.

The energetic and technical energetic establishment maps based on the distance observation aerospace method of the territoty prove that towel solar power stations may be developed and applied on the higher mountainous area where solar energy potential is more. Solar plate collectors and PVs can be utilized in both potentials, thus in the middle and the low potentials mostly at the house, schools, kinder gardens, hospitals, farms and others.

Thus, from the ecoenergetic and ecoeconomic points of view the local solar energy potential is effective to stop the deforestation process in the Mountainous Shirvan agroecological region. By this way one main part of the historical woodland aerial on the Great Caucases could have been saved beforehand.

ELECTRICAL PROPERTIES OF Cd_{1-x}Fe_xTe THIN FILMS

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Semimagnetic semiconductors (SMSC) are solid solutions with a fraction of the cations replaced by the magnetic transition metal (TM) ions like Mn, Cr, Fe, Co and other rare earth metals. The great interest in studying the SMSC is stimulated by their unique electronic, magnetic and magnetooptical properties. For example, the band gap and the lattice parameters can be varied by changing the composition.

II–VI semiconductors have a greater dopant concentration of TM and have smaller defect concentration compared with III–V based semiconductors. II–VI based SMSC have been investigated extensively. Among II–VI semiconductors, CdTe is a good candidate as host material for SMSC. Most of the SMSC compounds grown and studied by using Mn as the substitutional magnetic ion, but the literature reports on Fe based SMSC are meager. The investigations devoted to Cd_{1-x}Fe_xTe SMSC is limited to the preparation characterization of CdFeTe thin films by various techniques. This paper reports the crystal growth of Cd_{1-x}Fe_xTe ($x=0.01\div0.03$) thin films, the results on growth mechanism studies, structural and electrical investigations.

Cd_{1-x}Fe_xTe (x=0.01÷0.03) SMSC thin films of thickness 1.5 µm were grown on cleaned glass substrates at the rate of u=18-20 Å/s by an molecular beam condensation technique in a 10⁻⁴ Pa vacuum. All technical details of the preparation methodology were given in our earlier works. The structure and phase purity of thin films were checked at room temperature by means of *X*-ray powder diffraction (XRD) using a BRUKER XRD D8 ADVANCE. It was defined a phase transition from amorphous to crystalline phase in the substrate temperature range 570–620 K.

Electrical resistance measurements of $Cd_{1-x}Fe_xTe$ ($x=0.01\div0.03$) thin films were studied in the temperature range 100–500 K. At 300 K temperature, the resistivity of the $Cd_{1-x}Fe_xTe$ ($x=0.01\div0.03$) thin films was in the range of ($0.5\div2.5$)10⁶ Ω . Thin films exhibited *p*- type conductivity. Resistivity decreases with increase in temperature. The resistivity decrease with increasing of Fe concentration. The room temperature resistivity decreases almost linearly with Fe content. The decrease in resistivity with increasing Fe concentration in the thin films can be explained by the magnetic *d* states in SMSC, which appear near the Fermi level. The states may exhibit splitting, resulting in higher spin configuration of *d* electrons. The impurity states undergo hybridization with *p* states. The *d* state of Fe split under the influence of tetrahedral crystal field of CdTe. With the increase in temperature the electrons in the impurity states jump into the conduction band due to thermal activation. This explains the observed decrease in resistivity with increase of temperature. CdTe is a wide band gap semiconductor material. With increase in Fe concentration in the CdTe, more number of electrons is promoted to conduction band, resulting in further decrease in resistivity.

The decrease of resistivity with Fe concentration *x* is not uniform due to unknown different defect structures in thin films of different compositions. The resistivity and activation energy of the crystals were decreased with increasing Fe content.

KEYWORDS: Semimagnetic semiconductors, thin films, XRD, resistance, concentration.

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THERMAL CONDUCTIVITY AND THERMAL DIFFUSIVITY DATA OF FLUIDS WITH THE TRANSIENT HOT-WIRE TECHNIQUE

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Academic research laboratories and industrial research and development laboratories are in high demand of accurate thermophysical properties' measurements of fluids in a wide temperature range. Especially thermal conductivity measurements at temperatures below 0 °C are difficult to achieved because of the temperature instability of the temperature devices. In addition, the combination of systems that allow high and low temperature measurements are in many cases difficult because require lots of devices and laboratory space.

The transient hot-wire technique is a primary method for the measurement of the thermal conductivity of fluids over a wide temperature and pressure range. For the present work a single-wire commercial device was used to measure the thermal conductivity, thermal diffusivity and volumetric specific heat for common liquids.

The THW-L1E device is suitable for thermal conductivity measurements of fluids from -100 °C to 300 °C under pressures up to 35 bars. The transient hot-wire sensor allows measurements from 0.01 to 2 W/m·K with an uncertainty of 5% and repeatability of better than 1%.

To investigate the correct operation of the device through the whole temperature range Water, Heptane, Toluene, Isopropanol, Methanol, Ethylene glycol, and Glycerol measured. Around the melting/freezing point of the sample the anomalous thermal conductivity results can me noticed. Back pressure applied on the fluids allowed thermal conductivity measurements above their boiling point.

All the measurements were controlled through the user friendly THW software which shows to the user the measurements quality, suggests changes and export the data for further analysis.

MEASUREMENTS AND MODELING OF THERMODYNAMIC PROPERTIES FOR THE CYCLOALKANES

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Today's world is aiming for carbon neutrality, and hydrogen is one of the keys that will be used to achieve this goal. Hydrogen allows the capture, gathering, and storage of renewable energies. Various hydrogen carriers have been recently suggested for the worldwide transportation of hydrogen. Our work supports the development and control in hydrogen reforming processes based on hydrogen carriers through the use of precise measurement and modeling of the thermodynamic properties of the pure fluids and their mixtures. In this presentation, the current development of the preliminary thermodynamic property models for cycloalkanes, for example, cis-decalin and methylcyclohexane that are the main components in the hydrogen reforming process, will be reported. Measurements were made in the high temperature range of the hydrogenation and dehydrogenation process (which is commonly higher than 573 K) with the use of a modified metal-bellows volumetric apparatus for temperatures up to 600 K. The expanded uncertainties (k=2) in temperature, pressure, and density measurements of the apparatus have been estimated to be less than 5 mK, 0.02 MPa, and 0.88 kg/m³ (except the higher temperature and pressure ranges above 423 K and above 100 MPa, where the density uncertainty increases to 2.94 kg/m³). Throughout the fitting process of the Helmholtz energy equations of state, we adopted the most up-to-date constraints to appropriately modify the numerical values of the coefficients and exponents in the equations and the behavior of various derived properties, for example, the isobaric specific heat capacity, C_P, and Phase Identification Parameter, PIP, to assure thermodynamic consistency over the entire fluid-phase region.

SURFACE TECHNOLOGY AS A KEY TECHNOLOGY FOR ENERGY SYSTEMS

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Siemens Energy is one of the world's leading energy technology companies. The company works with its customers and partners on energy systems for the future, thus supporting the transition to a more sustainable world. With its portfolio of products, solutions and services, Siemens Energy covers almost the entire energy value chain – from power generation and transmission to storage. The portfolio includes conventional and renewable energy technology, such as gas and steam turbines, hybrid power plants operated with hydrogen, and power generators and transformers. More than 50 percent of the portfolio has already been decarbonized. An estimated one-sixth of the electricity generated worldwide is based on technologies from Siemens Energy.

Using renewable electrical energy like wind or solar power for "green electrons" from the power sector to decarbonize energy across all sectors unlocks enormous environmental and business benefits. Through Power-to-X technologies, sectors beyond power generation will benefit from renewable power and become increasingly green over the total chain from production to application.

Siemens Energy will provide optimum solutions in order to contribute to the realization of a carbon-neutral society in countries and regions around the world by utilizing our hydrogen related technologies, business and global network. The joint vision of the two companies is to advance the technology to produce green hydrogen from innovative PEM (Proton Exchange Membrane, Fig.1) water electrolysis using renewable energy systems. PEM water electrolysis (Fig.2) enables the production of high-purity green hydrogen. The resulting green hydrogen can not only be used for large-scale power generation and other electric power applications, but also for sector coupling such as heat, transport, and industrial applications.







Figure 2: PEM Water Electrolysis (Silyzer 300)

An PEM-electrolysis cell consists of a MEA (Membrane Electrode Assembly; Catalyst Coated Membrane) as well as porous structures (gas diffusion layer & fleece) on both sides for the distribution of product gases. The cells are separated in the segment by bipolar plates.

The PEM-systems have been further developed regarding efficiency, service life and cost-effectiveness. The key performance indicators (KPIs) of an electrolysis stack can be derived from the current-voltage and voltage-time curves.

Customized development of new energy innovative systems, like PEM-electrolysis are possible thanks to leading key enable technologies, e.g. surface technology. Surface and coating are relevant design elements for efficient product development for energy systems. For enabling multifunctional properties of components for energy systems, close cooperation between customer, application, research institutes, production is the key for success.

THERMOPHYSICAL BEHAVIOR OF CHOLINE CHLORIDE BASED DEEP EUTECTIC SOLVENTS WITH WATER AS NEW WORKING FLUID FOR AN ABSORPTION HEAT TRANSFORMER

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The High price and toxicity of ILs, and the harsh organic solvents has led to the discovery of deep eutectic solvents (DES). DES are now rapidly emerging in numerous applications owing to their green character, biodegradability, tenability, low cost and simple preparation, compared to other solvents. The possibility that natural DES might play a role as an alternative media in industrial processes pushed the researchers to investigate their use as solvents in heat absorption transformers.

In this work, thermophysical properties including vapor-liquid equilibria, heat capacity, density and excess molar enthalpy of binary mixture composed of $\{H_2O + g|yceline\}$ were measured at different temperatures and in a large range of composition. Then, experimental data were used to simulate the performance of absorption heat transformers using this binary system as working fluids. Simulation results show that binary systems containing glyceline and water are adequately suited for industrial absorption heat transformers.

MODIFIED HIND UBBELOHDE APPROACH FOR VISCOSITY PREDICTION FOR BINARY AND TERNARY LIQUID MIXTURES

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Viscosity has proven to be the transport property that has gained a significant role in the study of intermolecular interaction in multicomponent liquid mixtures owing to its multifarious industrial applications. Studying predictive equations is vital as it reduces the expenditure on expensive experimental setups and for being time-consuming. A perusal of literature reveals that the Hind Ubbelohde equation is a very basic and elementary predictive model for viscosity prediction. In the present investigation, we have attempted to modify the Hind Ubbelohde approach by introducing a volume fraction-based approach. This proposed approach has been put to test on 175 binary, 15 ternary, over a wide range of temperatures. A Comparative study has been carried out employing established predictive equations using average Absolute Percentage Deviation (AAPD) as a criterion for prediction. Grand AAPDs highlight the performance of the proposed approach in comparison to its original counterparts.



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SO MANY DATA, SO LITTLE INFORMATION? ON THE POTENTIAL OF MONITORING SYSTEMS AND PREDICTIVE MAINTENANCE IN THERMAL POWER PLANTS

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Expert systems and predictive maintenance are known in thermal power plants for many decades. At the end of the seventies and the beginning of the eighties, especially operators of nuclear power plants noticed the potential of using available data to increase profitability of their power plants by reducing operational downtimes and reducing maintenance costs [1]. Although computational power was limited at this time, artificial intelligence was already mentioned [2]. In the upcoming years, predictive maintenance was reported occasionally for different use cases in coal fired and gas fired power plants, micro-gas turbines or solar thermal power plants. However, a systematic search in ScienceDirect and Web of Science with the terms "predictive" AND "maintenance" AND "power plant" results only in 195 papers which is a rather low number compared to other research areas. One major reason for this was already mentioned: the high costs of computational power at least until the end of the nineties. Even with computational power getting cheaper and cheaper, a widespread use of available data for predictive maintenance has not taken place yet.

In our contribution we provide insights in an online monitoring system of a biomass fired power plant with a nominal electric power of 8.1 MW and a firing capacity of 40.5 MW. We present the present data acquisition and preprocessing steps necessary to develop and apply an online monitoring system that is combined with algorithms for predictive maintenance. The potential but also the limitations of such a system is shown for different subsystems of the power plant including the water treatment system but also the firing in combination with the turbine output. Furthermore, preliminary steps towards and automated monitoring system based on a cloud system of our project partner Gantner Instruments and applied on a power plant of our second project partner BertschEnergy are discussed. With this contribution we aim to show that computational power, data availability and expert knowledge would be ready for a widespread use of predictive maintenance in thermal power plants.

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THE STUDY OF HEAT CAPACITY AND THERMAL EXPANSION OF BISMUTH IRON PHOSPHATE

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BiFe₂(PO₄)₃ is promising material in the light of its interesting magnetic and dielectric properties. It shows typical antiferromagentic type behavior below 22 K. Given the potential applications of the phosphate, it is necessary to know its thermal behavior and thermophysical properties.

Polycrystals of the BiFe₂(PO₄)₃ compound have been synthesized by evaporation of the salt solution followed by heat treatment. According to the DTA, XRD, and thermogravimetry data, BiFe₂(PO₄)₃ congruently melts at (1313 \pm 5) K.

X-ray and energy dispersive X-ray spectroscopy results confirmed phase purity and the stoichiometry of the phosphate to be close to the theoretical composition of BiFe₂P₃O₁₂. The compound crystallizes in the structural type α -CaMg₂(SO₄)₃, sp. gr. *P*6₃/*m*, *Z* = 6, *a* = 1.43115(4) nm, *c* = 0.74311(2) nm.

The studied $BiFe_2(PO_4)_3$ expands on heating with positive thermal expansion and is medium-expanding material (Table).

The phase transition observed at temperatures of 12–32 K is presumably related to the ordering of magnetic moments in the structure of the compound: $\Delta H_{tr} = 87.4 \pm 1.8 \text{ J} \cdot \text{mol}^{-1}$, $\Delta S_{tr} = 4.00 \pm 0.08 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. The standard entropy of BiFe₂(PO₄)₃ formation at *T* = 298.15 K was estimated to be (1464 ± 2) J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}.

Table. Thermal Expansion Coefficients for Compound BiFe₂(PO₄)₃ (173 \leq (*T*/K) \leq 473, p° = 0.1 MPa)

	thermal expansion coefficients/ α·106 K-1			
α _a	ac	α _{av}	av	
4.0	-3.1	1.6	4.8	

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ABOUT INTERRELATION BETWEEN PVT AND PHASE EQUILIBRIA IN THE SYSTEMS OF IONIC LIQUIDS

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Detecting the general regularities characteristic for various systems of ILs in wide range of conditions is an important step in developing the entirely predictive approaches for reliable estimating their phase equilibria. Such regularities can be revealed while bearing in mind that all parts of the thermodynamic phase-space are closely interrelated. In particular, the experimentally inaccessible critical data of ILs are supposed to be linked with their compressibilities.

The higher compressibilities indicate the closer proximity to the critical points. In other words, the higher dependence of densities on pressures are supposed to indicate the lower imaginary T_c and P_c values, and visa versa. These imaginary critical constants can be particularly important in the context of phase equilibria in mixtures. As the distance between the critical points of solutes and solvents increase, the systems become more asymmetric, both the VLE and the LLE ranges get wider, meaning thus the lower molar solubilities. Consequently, it can be demonstrated that the molar solubilities are related to the *PVT* of ILs. Besides that, phase equilibria are also influenced by the critical constants of the solvents. Their higher T_c and P_c values typically increase the symmetry and, therefore, the solubilities.

CP-PC-SAFT rigorously obeys the T_c and P_c of ordinary compounds and can precisely represent the densities of ILs in wide range of conditions. It is demonstrated that such features attach this model by a remarkable predictive potential even while neglecting the association and polar interactions occurring in the halocarbon-IL systems. In most of the cases CP-PC-SAFT with $k_{12} = 0$ correctly estimates the differences between phase equilibria in the considered halocarbon-ILs systems, while the quantitative agreement with the available experimental data is usually reasonably good as well.

THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF ALKANONE + AROMATIC AMINE MIXTURES AT THREE DIFFERENT TEMPERATURES

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Proteins are polymers of amino acids linked to each other by peptide bond. The study of these amino acids, amides, peptides and their derivatives are very interesting for knowledge of complex biological molecules. The carbonyl and amide group present in the Alkanone and Aromatic amine mixtures are of interest to study the effect on the interactions.

In the present investigation an attempt has been made to evaluate internal pressure (Pi), energy (ΔE_{vap}) and enthalpy of vaporization (ΔH_{vap}) and their corresponding excess parameters along with excess entropy for binary solutions of alkanone (2- Propanone, 2-Butanone, 2-Heptanone) and aromatic amines (Aniline, N-Methylaniline, Pyridine) at 293.15, 298.15 and 303.15 K. Coefficient of thermal expansion (α) and isothermal compressibility (β T) have been computed and subjected to extensive application to evaluate the aforementioned parameters. All the properties and their excess counterparts have been used to understand the nature of intermolecular interactions taking place.



Figure 1. Excess Internal pressure (P_i^E) vs. mole fraction (x_1) for binary solutions of Propanone and aromatic amines at 298.15 K.

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HEAT TRANSFER IN SUPERCRITICAL FLUIDS: NON-IDEAL CONDITIONS

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Due to the anomalous behaviour of thermophysical and kinetic properties of substances in the near-critical region, supercritical fluids (SCFs) have attracted considerable attention both in terms of their inherent interest to science and their various technological applications [1, 2]. In practical point of view, this observation fully applies to the development of power units based on supercritical heat carriers. Indeed, the prospects of SCFs are justified, since a boiling crisis is impossible at supercritical pressures ($p > p_c$, p_c is the critical pressure). Moreover, in *ideal-ized* experiments the thermophysical properties of fluids show extreme type of behavior directly in the near-supercritical region.

In recent years, a paradoxical problem appears to occur, when the notion of the peaks of thermophysical properties, known from stationary measurements, coexist with the results of pulse experiments performed in conditions of high-power heat release. These results obtained for "probe/SCF" system in the framework of the high-speed technique and based solely on comparison of the primary data indicate a threshold decrease in the intensity of heat transfer near the critical temperature [3]. An explanation of this situation becomes a fundamental scientific task. The aim of the present report is to summarize the results of pulse experiments performed in conditions of high-power heat release. The purpose of this summary is to suggest a relatively simple approach to reconciling the short-term results on *nonideal* system with the peaks of thermophysical properties derived from experiments in stationary conditions.

The conditions for short-term experiments should generate factors that can shake the dominant role of the peaks of thermodynamic and transport properties. It is reasonable to assume that a substance entering the region of near-critical values of temperature and pressure, which are set in the pulse experiments, does not pass into a critical state in the usual sense of the term. Under conditions of large values of the heat flux density and temperature gradient, as well as a short response time of the heat-transfer surface, the long-range critical correlations are not formed. Accordingly, anomalies of the properties well-known from stationary measurements do not manifest themselves.

Thus, application of a short-term technique for studying supercritical heat transfer has led to unexpected results capable of influencing the direction of future research on this subject. The short thermal relaxation time of the micro-sized probe allowed identifying heat transfer patterns at small characteristic times and sizes, as well as at high heat flux densities. The experimental conditions were found, accompanied by suppression of large-scale fluctuations in thermodynamically non-equilibrium system and, consequently, smoothing of the critical enhancement of the properties. It is to be supposed, that this circumstance is a fundamental factor in the emergence of the HTD mode, considered as an obstacle to the application of SCFs in the processes, in which high-power local heat release appears to be possible.

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HARVESTING OF TURBULENCE ENERGY BY MEANS OF PIEZO-ELECTRIC MATERIALS

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With the nowadays challenges facing the environment, it has become crucial to raise the efficiency of energy systems. Among the forms of energy that normally exist in the environment is the energy existing in air flow. Therefore, this work aims at studying the potentials of harvesting the energy existing in turbulent flow by means of piezo-electric transducers. The study is based on relating the amount of generated voltage to both of the Reynolds number as well as the resulting Strouhal number of the flow. The considered transducers have a cylindrical shape and are made of Lead Zirconate-Titanate (PZT). The cylinder is placed across an airflow such that the flow interacts with the cylinder surface changing the turbulence energy of the flow into electric energy. Several configurations are experimented where the cylinder is placed with an angle between the cylinder axis and the flow direction set to be 0° (axial flow), 22.5°, 45°,67.5° and 90° (cross flow). The flow has a controlled Reynolds number while the voltage generated on the cylinder inner and outer surfaces is measured over time by means of an Oscilloscope. Reynolds number is determined based on the far velocity of the airflow as well as the diameter of the cylindrical transducer. The study considered Reynolds number in the range of 1000 up till 15,000. By performing Fast Fourrier Transform (FFT) to the obtained voltage measurements over time, it was found that the voltage data achieves the Kolmogorov's five-thirds rule of energy dissipation in turbulent flow. Such an observation indicates that the harvested energy is analogues to the turbulent energy in the flow which proves the possibility of piezoelectric cylinders to harvest energy of the turbulent flow.

PHASE EQUILIBRIA AND THERMODYNAMIC PROPERTIES IN THE o-DICHLOROBENZENE – m-DICHLOROBENZENE SYSTEM

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The Rankine cycle is widely used in industry to convert heat to work using a working fluid. The efficiency of the process can be improved by using an organic working fluid. A mixture of *o*- and *m*-isomers of dichlorobenzene can act efficiently as such a fluid. In order to design the process correctly with a new fluid, it is necessary to predict correctly phase equilibria and properties of the phases. An equation of state (EoS) approach was chosen to model liquid and vapor phase properties, as well as to calculate vapor-liquid phase equilibria.

Some experimental data for the pure substances are needed to parametrize a model. The data were already available in the literature. Several different EoS were parametrized for pure substances. The best results were achieved with Tsai-Chen EoS. Experimental measurements of volumetric properties of mixtures (density measurements at 1 bar) and solid-liquid equilibria (differential scanning calorimetry) were performed. These data were correctly predicted within the ideal assumption. Fragment of phase diagram is presented in Figure 1.

A *h-P* diagram for the *o*-dichlorobenzene – *m*-dichlorobenzene system was calculated using the resulted EoS (Figure 2). The diagram can be used to estimate energy efficiency of plants operating on the Rankine cycle with an *o*-dichlorobenzene – *m*-dichlorobenzene working body.



Figure 1. Fragment of *o*-dichlorobenzene – mdichlorobenzene phase diagram: red circles – experimental values, blue square – estimation of eutectic composition by "enthalpic" method, lines – calculation under the assumption of an ideal solution.



Figure 2. *h-P* diagram calculated for the *o*-dichlorobenzene – *m*-dichlorobenzene system.

A NOVEL METHOD FOR BINARY VAPOR-LIQUID EQUILIBRIA MEASUREMENTS

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Binary vapor-liquid equilibria measurements involving low-saturation-pressure solvents like ionic liquids are essential for designing processes in thermal separation, catalysis, fuel cells, carbon capture, refrigeration and more. Conventional methods to measure these phase equilibria like gravimetric microbalances or stoichometric pressure drop are limited in performance and speed, and cannot simply be combined with instruments measuring thermophysical properties. A novel method has been developed for efficiently measuring solubility simultaneously with other properties using the liquid density.

The governing equations will be presented and the method discussed and validated using gravimetric microbalance measurements obtained from refrigerant-lubricant mixtures. Simplifications will also be described that can be cost-effective solutions for specific measurement applications. The validated uncertainty in solubility of our initial realization of the method is around 0.2% with significant potential for optimization, extendibility and versatility depending on the application. Due to these advantages the novel liquid-density method will find wide application in many fields.

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PHONON TRANSPORT IN NANOFIBERS DOPED WIT GRAPHEN QUANTUM DOTS

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There is considerable interest to study the thermal transport in nanocomposites [1-2]. Nanocomposites with high thermal conductivity can be used to fabricate temperature-dependent nanodevices. These devices plays a significant role in integrated circuit chips which generate huge heat fluxes in extremely small areas. Hence, controlling heat fluxes in nanocomposites are very important for future generations of integrated circuits. Nanomaterials have also potential applications as electrodes in batteries, catalysts in microreactors and in fuel cell technology. Here we present a theory of the phonon transport for nanofibers doped with graphene quantum dots. We will calculate thermal conductivity with the Kubo formalism and the Green's function method. We will also calculate the density of states, phonon velocity and thermal conductivity. We have also applied our theory to explain the experimental thermal conductivity data of nanofibers. A good agreement between theory and experiments is achieved. Our results furthermore illustrate that one can fabricate new types of nanofibers with high and low thermal conductivity by adjusting the refractive index contrast between graphene quantum dotes and the host nanofibers. These nanofibers can be used to fabricate new types of thermal devices.

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MODELING OF SURFACE TENSION OF ORGANIC ACIDS USING A GROUP CONTRIBUTION APPROACH

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In recent years, the experimental determination and modeling of the surface tension of organic acids has received special interest due to its application in the design and simulation of equipment and processes such as the production of oils and biodiesel, synthesis and purification in the pharmaceutical and food industries.^{1,2}

In particular, the group contribution models offer different advantages for the prediction of surface tension of organic and inorganic compounds and they can be used with different approaches to improve their performances in the prediction of numerous families of compounds.³⁻⁵

Therefore, this study reports a set of surface tension models for organic acids based on a group contribution approach. These models require the temperature and molecular structure as input variables. A total of 870 experimental data point of 70 organic acids (including dicarboxylic, aromatic, aliphatic and polyfunctional) were utilized for determining the group contributions and testing the model performance. The group contributions were determined by minimizing the relative errors as objective function using Simulated Annealing-Quasi Newton method implemented in MATLAB software. Results showed that the best group contribution model showed a modeling error of $2.66 \pm 3.78\%$ with a determination coefficient of 0.99. A comparison was made with other four models reported in literature. It was concluded that our model outperformed other models reported in literature, which showed modeling errors up to 48%.

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DENSITY FUNCTIONAL THEORY STUDY OF THE ADSORPTION MECHANISM OF ANIONIC DYES ON CARBON SURFACES

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Density functional theory (DFT) calculations were computed to understand and characterize the adsorption mechanism of acid blue 80, acid blue 113 and acid blue 129 dyes on carbon surfaces. Specifically, the contribution of six different adsorbent functionalities (carboxylic acid, phenol, lactone, amide, chromene and carbonyl species) on the removal of dyes was studied. DFT calculations were performed to characterize the dye molecular properties and the carbon surfaces atomic distribution. In addition, the reactivity of both dye and surface was computed via molecular electrostatic potential (MEP) to identify the proper atomic interactions. The information gathered via MEP showed that the most deficient electron regions were near to hydrogens, particularly near to the aromatic rings on the dyes, whereas the rich electron regions were near to sulfonate groups contained in the molecules. Moreover, for the carbon surfaces the most electron deficient regions are the aromatic rings, locating the rich electron region on the functional group attached to it. So, the interaction complexes must be formed directing the most electron deficient regions on the dye towards the functional group on the carbon surfaces to obtain a potential interaction adsorbate -adsorbent. Results showed that interactions for anionic dye adsorption corresponded mainly to an interaction between hydrogen atoms on the dye towards oxygen atoms on the adsorbent surface. Overall, DFT results indicated that there was a trend for the adsorption of the anionic dyes: AB129 > AB113 > AB80.

PREDICTION OF CRITICAL PROPERTIES AND NORMAL BOILING POINT OF PURE COMPONENTS USING GROUP CONTRIBUTION AND ARTIFICIAL NEURAL NETWORK MODELS

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The knowledge of the critical properties of pure components is required for the processes design, simulation, optimization and control. The experimental determination of critical properties is expensive and could imply challenges (e.g., some molecules can degrade before reaching the critical conditions) ^{[1].} Therefore, it is important to develop reliable thermodynamic models to predict these properties. Group contribution models (GCMs) have advantages to estimate critical properties of pure components ^[2]. Some models have been combined with artificial neural network (ANN) models to improve their performance ^[3]. However, GCMs show high modeling errors for certain components and they cannot estimate the properties of different molecules due to the absence of some group contributions ^[4]. To date, few studies have carried out reliable comparisons of the performance of different models to estimate the critical properties of pure components.

We report a comparative study of several first order GCMs to estimate critical properties and normal boiling point of pure components. The capabilities of these models for different families of chemical components were compared using a standardized and reliable methodology to determine the group contributions. In addition, an ANN model was used to improve the estimates obtained with the GCMs. Results indicated that the easiest property to be predicted was the critical volume, while the most difficult one was the critical temperature. The highest modeling errors were obtained in the prediction of thermodynamic properties of alkanes, nitrogen, organosilicon and halogenated components and for molecules with high and low molecular weights within a homologous series. The ANN model improved the estimates obtained with the classical GCMs. The models obtained in this research showed a better performance to estimate normal boiling point, critical pressure and critical volume than those reported in the literature. These results can be used to establish strategies to improve the capabilities of thermodynamic models in the prediction of pure components properties.

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FLUCTUATION MODEL FOR PREDICTING THE HEAT CAPACITY OF NANOFLUIDS ON THE BOILING LINE

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The paper provides a critical analysis of the existing methods for predicting the properties of substances on the boiling line. The characteristic specificities that hinder the development of models for predicting the thermodynamic properties of nanofluids are considered. The effects of various nanoparticles on the thermodynamic properties of nanofluids, which can be both colloidal and molecular solutions, are analyzed. It is shown that most of the existing methods for calculating the heat capacity of nanofluids on the boiling line do not take into account the effects of structural changes in the liquid phase of substances in a wide temperature range.

To solve the problems of predicting the heat capacity of nanofluids on the boiling line, the authors propose to study the dependences of the heat capacity of pure substances and nanofluids on the boiling line on the isothermal compressibility coefficient and mean squared (rms) volume fluctuations.

The paper provides a detailed analysis of the temperature dependences of the isothermal compressibility coefficient and rms volume fluctuations for various classes of substances. It is shown that the considered temperature dependences in logarithmic coordinates for thermodynamically similar substances are equidistant lines. The performed research allows us to formulate a conclusion that the proposed principle of determining the thermodynamic similarity of substances can be applied also to nanofluids. The analysis of the published data on the heat capacity of nanofluids shows that thermodynamic similarity is observed for those objects of study, whose temperature dependence of the isothermal compressibility coefficient and rms volume fluctuations are equidistant lines. Thus, the availability of information on the temperature dependence of the isothermal compressibility coefficient and rms volume fluctuations can be the basis for the development of a universal method for predicting the heat capacity of nanofluids. Such information can be easily obtained from the data on the density of nanofluids on the boiling line with the subsequent calculation of the isothermal compressibility and volume fluctuations using the Kesselman equation of state.

The paper proposes a method for predicting the heat capacity on the boiling line of nanofluids using data on the density of various nanofluids as initial information. The results of justification of the proposed method are analyzed.

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PRODUCTION OF THERMOPLASTIC BASED COMPOSITE MATERIALS WITH AGRICUL-TURAL WASTES, IMPROVEMENT OF THEIR MECHANICAL AND THERMAL PROPERTIES

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Plastics are used in almost many sectors today. Thermoplastic-based composites with various properties such as mineral filled composites are frequently preferred in many industries. Mineral filled composite materials pose a potential danger to the environment due to synthetic origin of both polymeric matrix and filling material. In recent years, the use of sustainable and green polymeric composites have gained importance in order to minimize the environmental hazards. In order to achieve this goal, studies have been conducted on the development of bio-composite materials to increase sustainability by minimizing the hazards caused by synthetic origin. In this study agricultural wastes such as almond shell, rise husk, apricot kernel shell, pomace and thyme were added to poly-propylene matrix at a ratio of 20 wt.% and bio based (agricultural based) composite materials were produced by using a twin screw extruder. Test samples required for characterizations were obtained by using injection molding. Density, tensile, flexural and Izod impact tests according to ISO standards were performed for the samples. It was observed that approximately 10 percent weigth was saved in comparison with inorganic mineral filled polypropylene composites. By using agricultural wastes, green and environmental friendly composite materials have been obtained without any noticeable decrease in mechanical properties.

KEYWORDS: Polypropylene, agricultural waste, composite, sustainability.

Flash Presentations

STUDY OF AMIDOAMINES OBTAINED ON THE BASIS OF NATURAL PETROLEUM ACIDS AND POLYETHYLEPOLYAMINE AS ROAD BITUMEN EMULSIFIER

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It is known that emulsifiers are surfactants ensuring production of emulsions and stabilizing normally immiscible mixture of substances. Emulsifier molecules have an elongated shape with a hydrophilic and lipophilic terminals. Due to the structural characteristics, form a thin layer between the phases and are located at oil-water phases separation prevent droplets coalescence. Chemically, emulsifiers are anionic, cationic and non-ionic.

Bitumen emulsions provide an alternative approach that allows bitumen to soften by dispersing in water. Road bitumens are durable if the emulsion breaks down in the absence of water. The use of emulsions in road construction is safer and more environmentally friendly than hot bitumen. Bitumen emulsions are of great importance as a coating between the substrate and asphalt concrete.

Bitumen emulsifiers are almost not produced in our country and neighboring countries. Emulsifiers imported from abroad are very expensive. From this point of view, the creation of emulsifiers based on local raw materials is of great importance in our country, such as acid amines, organic acids, most of their metal salts, amidoamines, etc. Thus, synthesis of amidoamines on the basis of natural petroleum acids (NPA) and polyethylenepolyamine (PEPA) and testing as emulsifiers is of great scientific and practical importance.

In view of the above, amidoamines on the basis of NPA and PEPA (1:1 mol) were synthesized, their physicochemical properties were studied and tested as bitumen emulsifiers. For this purpose, the complexes were prepared on the basis of synthesized amidoamines and HCI in the ratio of 1:1-1:5 mol. The prepared complexes were added to the bitumen-distilled water mixture taken in a ratio of 1:1 by weight in different concentrations (0.5, 1, 1.5, 2 wt. %) and mixed at 80°C for 1 h. Further, the samples were tested in every hour to determine the duration of water separation. The best results were obtained in 2-4 pH range of emulsifier and 1.5 wt. % concentration of emulsifier to bitumen. That is to say, a satisfactory result was obtained in an acidic medium. Thus, in this case, 1-12 h later, breakdown of emulsion and separation of water didn't occur in 1.5 wt. % concentration of emulsifier to bitumen. The amount of water released after 1 day was ~ 8-10%. Thus, the synthesized amidoamines can be used as bitumen emulsifiers. Studies in this field are continued.

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INVESTIGATION OF THE PROCESS OF LIQUID-PHASE OXIDATION OF OIL DISTILLATE T-46

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The high demand for petroleum acids, limited natural resources and their presence in the form of complex mixture make the researchers on the synthesis of synthetic petroleum acids relevant. Thus, obtaining synthetic organic acids with higher performance characteristics is very important for petrochemistry and organic synthesis. In this regard, the development of various catalytic systems for the synthesis of mixture of synthetic acids based on the mineral oils of Azerbaijan, the development of high-performance mixture of synthetic acids with the participation of these catalytic systems and the creation of high-quality and industrial products based on the obtained acids are of great scientific and practical importance. This thesis is devoted to the synthesis of a mixture of petroleum acids by liquid-phase oxidation of oil distillate T - 46. The oil distillate was previously dearomatized [1]. The process of liquid-phase oxidation of T-46 oil was studied for the first time. Oxidation reactions of purified distillate T-46 were carried out in the presence of reduced graphene oxide as a catalyst, in an amount of 0,4 wt.% with respect to the feed, with a reaction time of 6 hours with a temperature of 180-190°C and the results are presented in the table.

Table 1. The results of liquid-phase oxisdation of oil distillate T - 46

The reaction prod- ucts	Yield, %	Acid number, mg KOH/g
SPA	38,7	155,8
OSPA	5,2	135,8
Oksidat	85	35,2

The yield of synthetic petroleum acids (SPA) resulting from oxidation is 38,7 wt.%, with an acid number of 155,8 mgKOH/g; the oxysynthetic petroleum acids (OSPA) is 5,2 wt.% with an acid value of 135,8 mgKOH/g; the yield of oxidat - 85 wt.% with an acid value of 35,2 mgKOH/g.

The mixture of acids obtained as a result of liquid-phase oxidation of T-46 oil in the presence of reduced graphene oxide was studied spectroscopically method and it was proved by the absorption bands that the resulting product is an acid.

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USE OF GLYCEROL ETHERS AS A LUBRICANT ADDITIVE TO DIESEL FUELS

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Production of low-sulfur diesel fuels requires improvement of their lubricating properties, as in the process of hydrotreating the compounds that provide the lubricating properties of fuels (sulfides, disulfides, benziophenes, etc.) are removed from the fuel and as a result, its lubricating properties deteriorate sharply. It should be noted that the lubricating properties of low-sulfur diesel fuels cannot be regulated by changing the technology of their production. The solution to this problem is the use of special anti-friction additives and fuel components.

In this study, mono-oleate and mono-acetate esters of glycerol, a by-product of the biodiesel production process, were studied as an anti-corrosion additive. The results are presented in Table 1.

Table 1.Dependence of the diameter of the wear stain on the concentration of glycerol mono-oleate and monoacetate esters in diesel fuel

concentration of glycerol mono- oleate and glycerol mono-acetate esters, m.h.	Diameter of wear stain, mkm	Decrease of wear stain diameter according to initial diameter%,		
0	850	0		
glycerol mono-oleate ether				
25	650	23,6		
50	515	39,4		
75	440	48,2		
100	400	53,0		
glycerol mono-acetate ether				
25	720	15,3		
50	645	24,1		
75	567	33,3		
100	500	41,2		
125	452	46,8		
150	430	49,4		

As can be seen from Table 1, the concentration of glycerin mono-oleate ether used to bring the wear stain of diesel fuel to the standard requirements is 0.0075% blunt. contane. At the same time, the diameter of the wear stain decreased by 48.2% to 440 microns.

In contrast, in the use of glycerin mono-acetate ether, the wear stain of less than 460 μ m is only 0.0125% blunt of this ether can be obtained in the presence of.

THERMOPHYSICAL PROPERTIES OF {[xCO₂ + (1-x)[EMIM][CH₃SO₃]} AND {[xCO₂ + (1-x)[BMIM][PF₆]} AT HIGH PRESSURES AND WIDE RANGE OF TEMPERATURES: CO₂ SOLUBILITY

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The greenhouse gases absorb infrared energy radiated from the earth, which results in an increase in the temperature of the troposphere. One of the most important greenhouse gases is carbon dioxide (CO_2). The continued burning of fossil fuels also will continue to increase CO_2 in the atmosphere, which cause worldwide climate change aka global warming and acidification of the environment. Thus, CO_2 removal from fuel gases has been a crucial technique for the availability of the fuel sources.

lonic liquids (ILs) have a stable liquid phase and low vapor pressure at room temperature. ILs have been suggested as potentially "green" replacements for conventional organic solvents since they are nonvolatile, nonflammable, thermal stable, and recyclable. They have also an excellent thermal and chemical stability. Recently, significant progress has been made in the application of ILs in various branches of industry, one of them as alternative solvents for carbon dioxide (CO₂) capture due to their unique properties.

In the literature many possibilities for carbon capture and sequestration are discussed. Many methods require the capture of CO_2 from e.g. the atmosphere or from combustion exhaust gases. This capture can be done by solution of the CO_2 in substances, e.g. in liquids, and especially in ILs. The prediction of gas solubility in ILs is a fundamental step toward the development of simulation tools to aid in the process calculations prior to industrial applications.

In this work, solubility data of carbon dioxide (CO₂) in the ionic liquids 1-ethyl-3-methylimidazolium methanesulfonate [EMIM][CH₃SO₃] and 1-butyl-3-methylimidazolium hexafluorophosphate [BMIM][PF₆] at T = (273.15 to 413.15) K and pressures up to p = 4.5 MPa will presented. The solubility measurements were carried out using an isochoric method which operates in decrements of $\Delta T = 20$ K within the investigated temperature range and at selected four different pressure steps ranging from a pressure p of around 5.0 MPa down to around 0.4 MPa. The solubility of CO₂ in the ionic liquid monotonously decreases with increasing temperatures at a constant pressure. Henry's law constant was calculated from the solubility data reported here, and literature data were reviewed for comparison. Additionally, thermodynamic state properties that can be derived from Henry's law constant, such as the Gibbs energy of solvation $\Delta_{sol}G$, the enthalpy of solvation $\Delta_{sol}H$, the entropy of solvation $\Delta_{sol}S$, and the heat capacity of solvation $\Delta_{sol}C_p$, were calculated.

Using the experimental solubility values the Henry's constant, the free energy of solvation $\Delta_{sol}G$, enthalpy of solvation $\Delta_{sol}H$, entropy of solvation $\Delta_{sol}S$ and heat capacity of solvation $\Delta_{sol}C_p$ were calculated at various temperatures.

SECTION (5Cu₂S)_{0,50}(7,5FeS)_{0,50}–(5Cu₂S)_{0,16}(3In₂S₃)_{0,84}

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The study of the nature of the chemical interaction between the chalcogenides Cu₂S, In₂S₃, FeS, as well as the study of the non-rotary properties of the obtained new phases is of great scientific and practical interest.[1,2]

This report presents the results of studying the $(5Cu_2S)_{0,50}(7,5FeS)_{0,50}-(5Cu_2S)_{0,16}(3In_2S_3)_{0,84}$. The system was studied using well-known methods of physicochemical analysis: differential thermal (DTA), X-ray phase (XRD), microstructural (MSA) analysis and microhardness measurement. Based on the results of DTA, it was revealed that the interaction between $(5Cu_2S)_{0.50}(7.5FeS)_{0.50}$ and $(5Cu_2S)_{0.16}(3In_2S_3)_{0.84}$ is complex. The study of the microstructure showed that, with the exception of some compositions, all alloys in the system are three-phase. When measuring the microhardness of individual phases of the system, several series of values were obtained. XRD confirmed the data obtained by MSA and microhardness measurements.

Taking into account the results of DTA, MSA, XRD and measurements of the microhardness of the samples, the phase diagram of this system was constructed, which is a non-quasi-binary section of the ternary system $Cu_2S - In_2S_3 - FeS$ [3,4].

The section crossed the fields of the subordinate ternary systems Cu₂S–CulnS₂–FeS, CulnS₂–CuFeln₃S₆–FeS, CulnS₂–CuFeln₃S₆–FeS, CulnS₂–Cu₃In₅S₉–CuFeln₃S₆; Cu₃In₅S₉– CuFeln₃S₆ –Feln₂S₄ μ CulnS₂–Feln₂S₄–Culn₅S₈. Therefore, its phase diagram consists of five independent parts. The liquidus of the section is represented by four branches of the primary separation of the α , γ , σ , δ - phases. A part of the section went through the subordinate ternary system Cu₂S–CulnS₂–FeS in the concentration range 0–61 mol.% (5Cu₂S)_{0,50}(7,5FeS)_{0,50}. There was one ternary eutectic (E₅) equilibrium at 990 K in this part of the section. The second part of the section crossed the secondary ternary system CulnS₂ – CuFeln₃S₆ – FeS in the range 61–79 mol.% (5Cu₂S)_{0.16} (3ln₂S₃)_{0.84}, where an invariant eutectic reaction is formed:

 $L \leftrightarrow \gamma(Culn_{S2}) + \gamma_1(FeS) + \delta (CuFeln_3S_6)$

In the range $79 \div 84 \text{ mol}\% (5Cu_2S)_{0.16} (3In_2S_3)_{0.84}$, crystallization ends in the ternary eutectic E₁ at a temperature of 1150 K. In the third part of the section, the crystallization of the alloys ends with the solidification of the ternary eutectic at the point E₂ at 1100 K.

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THERMODYNAMIC PARAMETERS OF Ni₃Sn AND (Ni₃Sn)_{0,99}Bi_{0,01} SOLID SOLUTION

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The Ni₃Sn compound is a stable phase in the Ni-Sn binary system, which melts congruently at ~1447 K, and has two modification transitions. The low temperature α -phase has an ordered structure with hexagonal crystal lattice of the Mg₃Cd type with parameters *a*=5.296 Å, c=4.242 Å, s/a=0.802. High-temperature modification has a crystal lattice of the Mg (A3) type and exists in the temperature range ~1194÷1447 K [1]. The microhardness of Ni₃Sn is ~4400 MPa. When revealing the nature of phase formation in the Ni₃Sn-Bi system, we discovered a region of solid solutions, the boundary of which at 300 K is 1.5 mol% Bi [2]. Therefore, it seems relevant to study the thermodynamic functions of (Ni₃Sn)_{0.99}Bi_{0.01} alloys.

If we calculate the atomization energy, we get that $\overline{H}_{S}(Ni_{3}Sn) = 398,65 \text{ kJ/mol}$. For solid solution $\overline{H}_{S}((Ni_{3}Sn)_{0.99}Bi_{0.01}) = 79,35$ kJ/mol. Taking into account the thermodynamic parameters of the individual elements [3] that make up the compound Ni₃Sn and the solid solution (Ni₃Sn)_{0.99}Bi_{0.01}, the values of standard heat capacity, enthalpy energy, free energy of formation of these compounds and solid solution are calculated. Using the Neumann-Kopp method [4], the specific heat of the Ni₃Sn compound will be C_p^0 (Ni₃Sn) = 105,59 J/(mol·K). For solid solution isobaric heat capacity $C_p^0 (Ni_3Sn)_{0,99} Bi_{0,01} = 104,79$ J/(mol·K). Using then Magnus-Lindeman equation [5], one can calculate the isochoric heat capacity of the Ni₃Sn compound. It was: $C_v^0(Ni_3Sn) = 105,04$ J/(mol·K). For solid solution, it was found that $C_v^0 (Ni_3Sn)_{0.99}Bi_{0.01} = 104,10$ J/(mol·K). The entropy can be determined by the Kelly method [4]: $\sum S^0(Ni_3Sn) = 141,71 \text{ J/(mol·K)}$, for solid solution $\sum S^0((Ni_3Sn)_{0.99}Bi_{0.01})$ = 140,86 J/(mol·K). The entropy of the Ni₃Sn compound and the solid solution based on it can be calculated using Hertz formula: $S_{298K}^{0}(Ni_{3}Sn) = 77,56 \text{ J/(mol·K)}, S_{298K}^{0}[(Ni_{3}Sn)_{0.99}Bi_{0.01}] = 77,65 \text{ J/(mol·K)}.$ The calculated entropies of formation of Ni₃Sn and (Ni₃Sn)_{0.99}Bi_{0.01} are: S_{298K}^{0} (Ni₃Sn) = -64,15 J/(mol·K). S_{298K}^{0} [(Ni₃Sn)_{0.99} Bi_{0.01}] = -63,21 J/(mol·K). The enthalpy of formation of Ni₃Sn can be taken from the [6], which has a value of -21.8 kJ/mol and using the Gibbs-Helmholtz equation, one can calculate the standard free energy of Ni₃Sn formation. Calculations showed that ΔG_{298K}^0 (Ni₃Sn) = -2,68 kJ/mol. If we take into account that the enthalpy of formation of elemental Bi is equal to zero and its quantity in the solid solution is negligible, then we can assume $\Delta H^0(Bi_{0,01})=0$. Then the free energy of formation of the solid solution will be $\Delta G_{298K}^0((Ni_3Sn)_{0.99}Bi_{0.01}) = -2,75 \text{ kJ/mol.}$

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INVESTIGATION OF COMPOSITIONS PREPARED ON THE BASES OF AMIDOAMINES OF SYNTHETIC PETROLEUM ACIDS AND MINERAL OIL DISTILLATES AS AN ADDITIVE TO BITUMEN

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It is known that the level of current development of the transport depends on continuous growth of the freight transport share, the movement intensity of the freight vehicles. This, in its turn, leads to the dynamic overload of the pavements. In accordance with the development of economy, demand on bitumen used in the road construction, and construction works are growing day by day. Therefore, enhancing the quality of bitumen is an important issue. High-quality bitumen must have adhesion property as a bonding material, resistance to formation of plastic deformation, as well as a wide range of plasticity to provide crack resistance at low temperatures, the properties in the high temperature range must be stable. Low-quality bitumen significantly reduces the service life of the pavement. Recently, there is a big order in the road construction, for the application of polymer-modified or polymer-bituminous adhesives (PBA) all over the world. We should mention that many adhesion additives are used in order to improve an adherence to gravel, i.e. an adhesion ability of bitumen. For this purpose cation-active surfactants – amidoamines, imidazolines, amine compounds and their salts are widely used.

In this regard, the compositions of different concentrations are prepared with amidomines obtained on the bases of synthetic petroleum acids (SPA) and polyethylenepolyamine (PEPA), and AK-15 motor oil, and the studies are conducted by adding these compositions in a certain percentage (0.4 and 0.6%) as an additive to bitumen. In purpose of enhancing the quality indicators of road bitumen, synthetic petroleum acids obtained from oxidation in liquid phase in the catalytic presence of transition metal salts of naphthene-paraffin hydrocarbons separated from the fraction of Azerbaijan petroleum mixture boiling at 185-330°C were taken as a raw material [1]. Amidoamines are obtained on known by using synthesized and PEPA. Amidoamines were obtained according to a known methodology using a mixture of synthesized SPA and PEPA in different molar ratios (SPA: PEPA = 1:1÷ 6: 1). The compositions of synthesized acids mixture in various percentage ratios (95-15%) with AK-15 motor oil have been prepared. The physical and chemical indicators of prepared compositions have been studied. These compositions have been used as a high-quality additive for road bitumen in purpose of enhancing the quality indicators of road bitumen. The compositions prepared on this purpose have been added to bitumen in amount of 0.4% and 0.6%, and the quality indicators have been compared with the quality indicators of the road bitumen produced at the Baku Oil Refinery named after H.Aliyev. It has been defined that an adhesion varies from 3 to 1 point by adding these compositions in small amount to bitumen. According to the quality indicators of bitumen, it can be mentioned that when the compositions of 0.4% prepared in concentration of 5÷15% on the bases of amidoamine, obtained from taking in molar ratio synthetic petroleum acids: polyethylene polyamines=5:1, and AK-15 motor oil added to bitumen at 25°C the values of penetration of 49-51 mm, extensibility up to >100 cm, brittleness temperature at interval of minus 22-27°C are obtained. It is defined that more positive results with enhancing the quality indicators significantly, are achieved in case of adding the composition of 0.6% obtained by taking amidoamine (90%) synthesized in molar ratios of synthetic petroleum acids: polyethylene polyamines=5:1 and AK-15 motor oil (10%) to the road bitumen

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STUDY AND MODELING OF THE PHASE DIAGRAM OF THE SYSTEM Bi₂Te₃-SnTe-PbTe IN THE REGION OF SOLID SOLUTIONS BASED ON SnTe, PbTe AND PERITECTIC PHASES SnBi₂Te₄, PbBi₂Te₄

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Bismuth, tin, lead tellurides and based on them ternary compounds are thermoelectric materials with low thermal conductivity, as well aspromising materials for creating topological insulators [1,2]. To date, the phase diagram of the Bi₂Te₃-SnTe-PbTe system has not been determined. This work presents the phase diagram of the Bi₂Te₃-SnTe-PbTe system in the region of the formation of solid solutions based on tin and lead tellurides, as well as peritectic phases based on SnBi₂Te₄, PbBi₂Te₄. The phase diagram was determined by complex methods of physicochemical analysis and modeled using the OriginLab computer program.



Figure. Phase diagram of the Bi₂Te₃-SnTe-PbTe system. α - solid solutions based on SnTe and PbTe. 1- liquidus surface; 2- border surface α -solid solutions; 3- plane of peritectic reactions of obtaining SnBi₂Te₄ and PbBi₂Te₄; 4 - plane for a mixture of SnBi₂Te₄, PbBi₂Te₄; 5- heterogeneous mixture of α - solid solutions and phases based on SnBi₂Te₄ and PbBi₂Te₄. Areas 1-4 are visualized with the following dependencies, respectively: 1) (1197-351*x-276.7*x^2-26.8*x^3)*y + (1079-

1) (1197-351 x-270.7 x 2-20.8 x 3) y + (1079-211.33*x-189,7*x^2-102.1*x^3)* (1-y)+16*y*(1-y); 2) (1197-1465.3*x+9728*x^2-91304* x^3) *y+(1079-1923.1*x+5841.7*x^2-6624.48* x^3)*(1-y)-48*y*(1-y) and 78+2563*x-3097*x^2; 3) 873-10*y; 4)-600+91000*(x-0,5). In equations (1-4): x= X(Bi₂Te₃); y= X(PbTe)/[(X(PbTe)+X(SnTe]; X_i- mole fractions Bi₂Te₃, PbTe and SnTe.

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ENVIRONMENTAL CONDITIONS AND CRIME SCENE: HOW TEMPERATURE AND HUMIDITY EFFECT BIOLOGICAL STAINS?

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In the crime scene investigation, the examination of biological stains such as blood, semen, urine, saliva or vaginal fluid is considered as important clues that potentially point out the perpetrator, the victim and the way the crime occurred. These stains may undergo metabolic or non-metabolic changes with the passage of time after their deposition.

Metabolic changes can occur by enzymatic and non-enzymatic pathways. Enzymatic changes occur especially in the early period. The speed and amount of these changes can be affected by the temperature and humidity changes of the crime scene. It is known that enzymatic degradation can come to a standstill in environments that are severely deprived of moisture. It is known that the activities of proteinases and DNAases increase in high humidity environments. Very low or very high temperatures can also cause metabolic changes to cease.

Non-metabolic changes often occur as a result of physical and/or chemical interactions. UV light and high temperature are the leading factors that damage the sample. Although degradation of protein structures is common at temperatures of 90 °C and above, high temperature also reduces the effect of washing to prevent the preliminary detection of stains. However, DNA extraction from these stains is also difficult. In this poster presentation, the global effects of temperature and humidity on the stains found at the crime scene were discussed.

KEYWORDS: Crime scene investigation, biological stain, humidity, temperature

THERMODYNAMIC PROPERTIES OF ETHANOL-WATER MIXTURE

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The model for ethanol-water mixture presented here is based on corresponding states theory and uses reducing parameters that are dependent on the mole fractions of the mixture constituents and critical points of the pure fluids to modify absolute values of the mixture density and temperature. The model uses the Helmholtz energy as the basis for all calculations. The Helmholtz energy of the mixture is calculated as the sum of an ideal gas contribution, a real fluid contribution, and a contribution from mixing. The Helmholtz energy from the contributions of the ideal gas and the real fluid behavior is determined at the reduced density and temperature of the mixture by the use of accurate pure fluid equations of state for the ethanol [1] and water [2]. Reducing parameters, dependent on the mole fractions of the constituents, are used to modify values of density and temperature for the mixture. The equation for the mixture Helmholtz energy used in this work is

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

where $\alpha(\delta, r, x)$ is the mixture Helmholtz energy; $\alpha^0(\rho, T, x)$ is the reduced Helmholtz energy in the ideal-gas state; $\alpha^r(\delta, r, x)$ is the residual part of the reduced Helmholtz energy; $\delta = \rho/\rho_r(x)$; $r = T_r(x)/T$; $\rho_r(x)$, $T_r(x)$ is the reducing parameters suggested by Kunz and Wagner [3].

The excess part can be defined by the following relation

$$\alpha^{r}(\delta,\tau,x) = \sum_{i=1}^{N} x_{i} \alpha_{0i}^{r}(\delta,\tau) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_{i} x_{j} F_{ij} \alpha_{ij}^{r}(\delta,\tau)$$
⁽²⁾

where $\alpha_{0l}(\delta, r)$ is the excess part of Helmholtz energy of component *i*; $\alpha_{ij}(\delta, r)$ is the excess function

$$\alpha_{ij}^{r}(\delta,\tau) = \sum_{k=1}^{K_{pol,ij}} N_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} + \sum_{k=K_{pol,ij}+1}^{K_{pol,ij}+K_{exp,ij}} N_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} \exp\left(-\delta^{l_{ij,k}}\right)$$
(3)

A nonlinear optimization procedure was used to develop mixture model. Optimization of the coefficients Eq. 3 took place simultaneously in a nonlinear form. The uncertainties of calculated values of various properties are determined by comparisons with experimental values.

Analysis of the literature data on the p, ρ ,T,x - properties of the ethanol + water mixture showed that most measurements were performed in the liquid phase at atmospheric pressure. For an objective selection of the most reliable and consistent experimental data for fitting pocedure, a local equation was developed that describes the density of the liquid phase at atmospheric pressure in the temperature range from freezing points to normal boiling points.

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THERMODYNAMIC PARAMETERS of AgCu_{1-x}Fe_xS COMPOUNDS UNDER NON-ISOTHERMAL CONDITIONS

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The study of the structure and thermal properties of condensed environments is one of the main research areas of modern crystallophysics and materials science. The results obtained from these studies play an important role both in explaining the various physical properties of existing compounds and in obtaining new composite materials based on them. Inorganic compounds with semiconductor properties are one of the most widely studied objects in modern electronics. It is well-known that one of the most important requirements for materials used in instrumentation is that they are temperature-resistant and, accordingly, have stable physical properties in a wide temperature range. Therefore, it is important to investigate the thermal properties of semiconductor compounds and determine the nature of phase transitions in the region of change of these properties.

In the present work, the AgCuS and with replacement Cu atoms by partial Fe atoms, AgCu_{0.99}Fe_{0.01}S, AgCu_{0.97}Fe_{0.03}S compounds were synthesized. By the differential thermal analysis method, the thermal properties of these compounds have been investigated, and in the high-temperature region the thermodynamic potentials for each system are determined.

For the synthesis of AgCu_{1-x}Fe_xS compounds ($0 \le x \le 0.03$), the sample weight was calculated by stoichiometric composition and placed in quartz ampoule, and the mouths of the ampules are soldered and rotating into the furnace. For the synthesis of compounds, B5 brand of Ag and Cu, B2 brand of Fe and sulfur were taken in special purity. Firstly, the temperature of the furnace was increased upto the sulfur melting point (T = 395 K). After being kept at that temperature for t = 4-5 h, which means, after the reaction of metals (Ag, Cu and Fe) with sulfur, the temperature increased to the melting temperature of the compound (T = 1410 K) and kept at the indicated temperature for t = 4-5 h, then the furnace was cooled with 60 °/h along with the ampoules. Microstructure, X-ray, phase microstructure, density determination methods (complex physical-chemical analysis methods) were used to check the purity of the compound. For homogenization of the synthesized compound, evaporated at temperature T = 450 K for 750 h then investigation was carried out. The phase analyses were performed on the D8 ADVANCE diffractometer using the X-ray diffraction method. Thermal properties of the AgCuS, AgCu_{0.99}Fe_{0.01}S and AgCu_{0.97}Fe_{0.03}S compounds were performed on a Perkin Elmer STA 6000 device at a temperature range T = 300-1300 K using the Differential Thermal Analysis Method. Measurements were made at a speed of 5 K/min. The cooling process was achieved with the help of the PolyScience analyzer cooling system and "digital temperature controller". The DTA spectra obtained in the high-temperature region were analyzed in Origin 9 software.

AgCu_{1-x}FexS crystals were synthesized at different concentrations of Fe atoms ($0 \le x \le 0.03$) and their thermal properties were investigated using a differential thermal analysis method at a temperature range of 300 K $\le T \le$ 1300 K. It was determined that phase transition in AgCuS and AgCu_{0.99}Fe_{0.01}S compounds occurs at the temperature $T \sim 940$ K. This phase transition in AgCu0.97Fe0.03S compound is not observed. In the AgCu_{0.97}Fe_{0.03}S compound, the phase transition occurred at $T \sim 1100$ K. The heat capacity and enthalpy values for each phase transition were calculated.

THE OXIDATION OF ALKANE C15 IN THE PRESENCE OF FULLERENE C60 TREATED BY ULTRASONIC

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Recent studies indicate an essential role of fullerenes in radical and electron scavenging reactions. These properties allow them to activate CH bonds in alkanes, followed by dehydrogenation [1,2]. These capabilities of fullerenes affect the growth dynamics of the formation of oxygen-containing products in the radical-chain process of hydrocarbon oxidation [3].

We carried out the reactions of liquid-phase aerobic oxidation of n-pentadecane in the presence of C_{60} fullerene, treated by ultrasonic, in a bubble-type glass reactor [3]. Fullerene C_{60} (8% content in the sample) was provided by the German company XzillionGmbH.

Ultrasonic treatment of the catalyst in hydrocarbon was carried out by cavitation unit «Hielscher» (Ultrasound Technology, production of Germany) UP200St (operational frequency -26 kHz), amplitude, which varies from 20% to 100%, impulsive operational cycle is V_{sec} , from 0,1 to 0,9, (Power) power of supplied ultrasound is equal to 200W)). In the cavitation process had been used titanium sonotrode s26d7 («Hielscher»), with a diameter of 7 mm and an amplitude equal to 190 μ m.

Table. Results of the oxidation of alkane C_{15} in the presence of fullerene C_{60} treated by ultrasonic (1 min) (T, $\circ C = 140$, τ of reaction, hour = 4.5)

Amount of	mount of USM A.n.		Yield of	Yield of	A. n. of	A. n. of					
cat.,		oxidate,	SFA, %	OSFA,	SFA	OSFA					
%	% mgKOH/g			%	mg	mg					
					KOH/g	KOH/g					
-	_	35.0	1.5	1.0	_	-					
0.0115	-	42.0	2	1	-	-					
0.0115	+	90.37	14	0.38	172.79	189.0					

A.n.. – acid number of oxidate, mgKOH/g; SFA- synthetic fatty acids; OSFA- oxy-synthetic fatty acids.

The results of studies on the liquid-phase aerobic oxidation of alkane C₁₅ in the presence of fullerene treated with ultrasound indicate:

- the catalytic activity of fullerene C₆₀ in the activation of C-H bonds in hydrocarbons;
- in the accelerated formation of oxygen-containing products in the process;
- the possibility of shortening the induction period due to the activity of fullerene C₆₀;
- the ability of fullerene to convert paraffinic hydrocarbons into synthetic fatty acids, preventing them from being converted into oxy-synthetic fatty acids;
- and with ultrasonic treatment, this activity doubles.

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STUDY OF RADIATION RESISTANCE OF SULFOCATIONITES

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At present, it is impossible to imagine an industry like nuclear technologies, and processes like the water treatment at thermal and nuclear power plants, purification of wastewater and coolants of nuclear reactors, etc. can be operated without of using of the ion exchangers. Basically, these processes are carried out at high temperatures or by influence of the ionizing radiation. With prolonged use of ion-exchange materials in these industries, they significantly change their characteristics and properties. It is known that the polymers' radiation modification ("crosslinking") leads to the formation of a spatial mesh in polymers, which significantly changes such characteristics of heat resistance, resistance to cracking, frost resistance, resistance to aggressive environment etc.

With intention to study changes in the main indicators of synthesized sulfonic cation exchangers, we carried out experimental work in this area. Sulfonic cation exchangers synthesized on the basis of a polymer mixture of wastes of polystyrene: polyvinyl chloride (WPS:PVC) taken in various ratios were subjected to radiation γ - irradiation with a cobalt source at the experimental base of the Institute of Radiation Problems of NASA in an aqueous medium at room temperature with an increase of the radiation from 10 to 50 Mrad. Pre-weigh 0,2-0,3 g of a sample of sulfonic cation exchanger, place in a lass test tube and seal the end of the test tube. Then the test tube is fixed to the stand, placed on the container and irradiated in the range from 5 to 50 Mrad.

After the experiments, such indicators of sulfonic cation exchangers as the swelling coefficient (K_{swelling}), static and dynamic exchange capacity (SEC and DEC), also mechanical strength were studied. Based on experimental data the radiation resistance of ion-exchange materials, it can be concluded that during irradiation, the static exchange capacity of the most ion exchangers decreases. The main reason of the decrease of the static exchange capacity and the deterioration of the operational properties is the elimination or destruction of functional groups, as well as weak crosslinking of the polymer structure. The destruction of the polymer matrix makes a significant contribution to the decrease in the exchange capacity and the swelling coefficient in aqueous solutions of the weakly crosslinked ion exchangers. In radiation chemistry, changes in the properties of ion exchangers are explained by both direct and indirect effects of radiation, i.e. absorption of radiation energy directly by functional groups. Below are the main indicators of sulfonic cation exchangers exposed to radiation-irradiation with a cobalt source.

	Table 1										
N⁰	Indicators of sulfonic cation exchanger based Before Radiation dose, MRad										
	on WPS: PVC (PVC content 2 parts by weight)	irritation	10	20	30	40	50				
1	Swelling factor	0,91	0,91	0,91	0,89	0,87	0,83				
2	Static exchange capacity of NaOH, mq-eq /g	6,2	6,2	6,0	5,9	5,7	5,3				
3	Dynamic exchange capacity of CaCl ₂ , eq /g	0,69	0,69	0,68	0,68	0,64	0,61				
4	Mechanical strength after 10 hours of shaking	90	90	90	88	88	88				

It is obvious from the table that irradiation of sulfonic cation exchangers in an aqueous medium at room temperature is accompanied by a change in the parameters of the exchange capacity and the swelling coefficient. Based on the data in the table, it can be concluded that at dose of up 15 Mrad, the proposed sulfonic cationites are resistant to radiation exposure and partically do not change their main parameters. With an increase in the irradiation dose to more than 15 Mrad, the static exchange capacity of sulfonic cation exchangers decreases. A gradual decrease in K_{swelling} and SEC indices of sulfonic cation exchangers with an increase in the absorbed dose indicates the destruction of the polymer base and partial destruction during irradiation. By increase of the irradiation dose, the sulfonic caionite samples become more fragile, which indicates a change in the mechanical strength.

A NOVEL AND SELECTIVE MULTI-EMISSION CHEMILUMINESCENCE SYSTEM FOR THE QUANTIFICATION OF DELTAMETHRIN IN FOOD SAMPLES

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A paper-based analytical device (PADs) combined with a powerful chemiluminescence (CL) system was established for the determination of deltamethrin (DM), based on the enhancing effect of polyphosphate (PP) on graphene quantum dots (GQDs)-KMnO₄ CL reaction. A possible mechanism for the obtained emission was proposed using the CL spectra, fluorescence and ultraviolet-visible patterns. The reaction of KMnO₄ and GQDs can lead to generation of GQDs in excited state (GQDs*), which can emit at 490 nm. Interestingly, PP changes the CL mechanism and the main emitter becomes Mn²⁺ instead of GQDs leading to a strong emission at 695 nm. Furthermore, the obtained multi-emission CL system was examined for analytical applications. The initial experiments showed that the amplified CL emission of the GQDs-KMnO₄ system was selectively quenched in the presence of trace levels of DM, probably due to its effective interaction with GQDs or reaction with KMnO₄. This observation led to a facile, reliable and sensitive PADs-CL probe, developed for the determination of DM residue in food samples. Using this CL system and under the optimized experimental conditions, the generated signal is decreased by increasing DM concentration in the range of 0.3–10 µg mL⁻¹ with limit of detection (LOD) of 0.15 µg mL⁻¹.

KEYWORDS: Chemiluminescence; Graphene quantum dots; Paper-based analytical device; Nanomaterial; Deltamethrin.

DESIGN OF NEW HYBRIDS ON THE BASIS OF SILVER NANOPARTICLES AND SALICYLALDEHYDE BASED SCHIFF BASES AND INVESTIGATION OF THEIR BIOLOGICAL ACTIVITY

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Schiff bases, which were first obtained by Hugo Schiff in 1864, are aldehyde- or ketone-like compounds in which the carbonyl group is replaced by an imine or azomethine group. Despite the fact that from the year of discovering more than 150 years passed, these compounds still don't lose their actuality due to their wide spectrum of application area. Along with their application in nanotechnology, organic synthesis, catalysis, they also demonstrate a broad spectrum of biological activity. Schiff bases have been investigated in relation to a wide range of contexts, including antimicrobial, antiviral, anticancer, antitumor, antiepileptic and anti-HIV activities. They have also been considered for the inhibition of amyloid- β aggregation and their activity can be used in the synthesis of a new generation of various drugs against diabetes.

From the other side, one of the promising biologically active components is silver nanoparticles. Along with its biological activity, it can be easily obtained and depending on reaction conditions size can be regulated. Another advantage is its dispersibility in water and other solvents.

Considering the positive sides of silver nanoparticles and Schiff bases, we synthesize new hybrids on the basis of mentioned components and investigate their activity against various gram-positive and gram-negative bacteria (S. aureus, E.coli, P. aeruginosa, A. baumannii, K. pneumoniae) as well as Verticillium dahleae fungus. For this purpose, first of all Schiff bases on the basis of (E)-2-(2-((2-hydroxybenzylidene)amino)ethoxy)benzaldehyde were synthesized by condensation with tris(2-aminoethyl)amine and 2 2'-(ethylenedioxy)bis(ethylamine). The structure of the obtained substances was confirmed by ¹H and ¹³C NMR and mass spectroscopy methods and elemental analysis. Next step was synthesis of Ag based ensembles, which structure and morphology were studied with TEM, XRD, and FTIR methods. Afterwards, biological activity investigations revealed promising results in comparison with the known antibiotics.



NEW VARIABLE COMPOSITION PHASES IN THE Ag, Ge || S, Te RECIPROCAL SYSTEM

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Due to interesting properties such as optical, thermoelectric, and photovoltaic, chalcogenides of silver with p²elements and phases based on them are among the perspective functional materials. Some of them have ionic conductivity and are prospective for use in various fields of modern electronics. The search and development of the foundations for new materials are based on reliable data on the phase diagrams of the corresponding systems. To obtain new phases with variable composition based on silver-germanium chalcogenides, this work presents the results of the phase equilibria investigations in the $6Ag_2S+Ag_8GeTe_6 \leftrightarrow 6Ag_2Te+Ag_8GeS_6$ (A) reciprocal system by using DTA (NETZSCH DSC 404 F1 Pegasus®), XRD (Bruker D8 ADVANCE diffractometer, Cu-K_{α} radiation), and SEM (Tescan Vega 3 SBH) methods.

The initial compounds were synthesized by fusion of high-purity elementary components in evacuated (~ 10^{-2} Pa) silica ampoules. The sulfide compounds were synthesized in a two-temperature furnace. Then by fusing the starting compounds also under vacuum, the samples of the system (A) were synthesized. After fusing all alloys were annealed at 800 K within 200 h. Then, a series of alloys was quenched in cold water, and the second series was cooled slowly to room temperature.

Based on the experimental results, the projection of the liquidus surface and isothermal sections at 300 and 800 K of the phase diagram of the system (A) were constructed (Figure). A continuous series of solid solutions (δ -phase) with a cubic structure is formed along the Ag₈GeS₆-Ag₈GeTe₆ section. At 800 K they form connodes with solid solutions based on the high-temperature cubic modification of the Ag₂S (α ₁-phase) and the intermediate cubic modification of the Ag₂Te (β ₁-phase).

The picture of phase equilibria at room temperature differs sharply from that at 800 K. Along the Ag₈GeS₆-Ag₈GeTe₆ section, the homogeneity region δ -phase based on Ag₈GeTe₆ narrows to ~45 mol%; based on the low-temperature orthorhombic modification, up to ~ 20 mol% solid solutions (δ_1 - phase) are formed. In addition, the Ag₄TeS (mineral cervelleite) compound and relatively narrow homogeneity regions based on low-temperature modifications of the initial binary compounds (α_2 - and β_2 -phases) are formed in the Ag₂S-Ag₂Te boundary system. The interaction of these phases leads to the formation of a number of two- and three-phase regions in the system (A). The obtained new phases are of great interest as potential materials with mixed ion-electronic conductivity.



 $6Ag_2S+Ag_8GeTe_6 \leftrightarrow 6Ag_2Te+Ag_8GeS_6$ system

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PHASE EQUILIBRIA AND SOLID SOLUTIONS IN THE Ag2Te-Ag8SiTe6-Ag8GeTe6 SYSTEM

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Compounds of the argyrodite family with the general formula A_8BX_6 (where A = Cu, Ag; B = Si, Ge, Sn; and X = S, Se, and Te) possess a number of valuable functional properties and are the subject of investigation by many research groups. In particular, due to their unique crystal structure, these compounds are typical superionic semiconductors and represent a promising class of environmentally friendly thermoelectric materials [1-4]. This work is devoted to investigation of phase relations in the Ag₂Te-Ag₈SiTe₆-Ag₈GeTe₆ (A) system.

All initial compounds of investigated system are characterized by polymorphism. Compound Ag_2Te has two polymorphic transformations above room temperature. Polymorphic transitions for ternary starting compounds of the system (A) are observed at temperatures below room temperature. High-temperature superconducting modifications for both Ag_8SiTe_6 and Ag_8GeTe_6 are crystallizing in cubic system. This allows expecting the formation of continuous or wide areas of solid solutions in the systems $Ag_8SiTe_6-Ag_8GeTe_6$.

Starting compounds were synthesized from high-purity elements (at least 99.999 wt.% purity) in sealed silica ampoules under vacuum (10⁻² Pa). Synthesis was carried out in a two-zone furnace. Samples of the systems were prepared by melting of the pre-synthesized compounds under vacuum also. Alloys were annealed at 900 K for about 500 h. Then one series of samples was quenched into water, and the second was additionally annealed at 400 K during 10 h.

DTA (NETZSCH DSC 404 F1 Pegasus) and XRD (Bruker D8 ADVANCE diffractometer, $Cu-K_{\alpha}$ radiation) were used to analyze the samples of the investigated system. Based on experimental data, the T-x diagram of the lateral system Ag₈SiTe₆-Ag₈GeTe₆ (Fig.), solid-phase equilibria diagram and the projection of the liquidus surface of system A were constructed. It was shown that Ag₈SiTe₆-Ag₈GeTe₆ section is guasi-binary and characterized by

formation of continuous series of solid solutions (δ -phase) with cubic structure. The dependence of the crystal lattice period of the δ -phase on the composition obeys Vegard's rule (Fig.).

It was found that the δ -phase is in a connode connection with all crystalline modifications of Ag₂Te, and thereby forming the corresponding two-phase areas. A liquidus surface of the system (A) consists of two fields corresponding to the primary crystallization of the HT-Ag₂Te and δ -phase. These surfaces are delimited by a eutectic curve characterized by monovariant equilibrium L \leftrightarrow HT-Ag₂Te + δ .



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THERMODYNAMIC PROPERTIES AND MODELLING OF TRICYANOMETHANIDE-BASED IONIC LIQUIDS WITH WATER

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In recent years, ionic liquids have attracted much attention as absorbents in absorption heat transformers due to their unique properties, such as negligible vapor pressure, nonflammability, thermal stability, low melting points, and liquid state over a wide temperature range¹. In this work, we present the experimental measurements of the isothermal vapor–liquid equilibria, densities, excess enthalpies and heat capacities of ionic liquids containing the same anions and different cations: 1-butyl-3-methylimidazolium tricyanomethanide, 1-butyl-4-methylpyridinium tricyanomethanide and 1-butyl-1-methylpyrrolidinium tricyanomethanide with water in a wide temperature range. Experimental data of vapor–liquid equilibria for water + IL systems were correlated using the Non-Random Two-Liquids (NRTL)². Excess properties were correlated using the Redlich–Kister equation. Furthermore, the effect of cations on thermodynamic properties was studied. In parallel COSMO-SAC and COSMO-RS models were used to predict vapor–liquid equilibria and excess molar enthalpy for such binary systems.

KEYWORDS: Ionic liquid, water, thermodynamic properties, NRTL, COSMO-RS models

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THERMOPHYSICAL AND CHEMICAL PROPERTIES OF GEOTHERMAL AND MINERAL WATERS OF AZERBAIJAN

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The thermal waters of tehse regions have high exiting temperature, high mineralization, which make them good candidates for using in domestic and medicine purpose. To use the thermal water resources in medicine, alternative heating source or domestic use, the investigation of the chemical and thermophysical properties of a wide range of parameters must be investigated can. In this work, the chemical and thermophysical properties of the following thermal waters of northern and southern Azerbaijan were studied.

Table 1. Investigated geothermal and mineral waters of Azerbaijan.

No	Thermal Water Samples	Latitude	Longitude
1.	Guba city	41°22′01.89"N	48°31′18.40"E
2.	Jimi 14 °C (near villiage Jimi)	41°02′20.78"N	48°32′54.38"E
3.	Jimi 65 °C (near villiage Jimi)	41°02′20.78"N	48°32′32.81"E
4.	II Nügedi village	41°19′00.00"N	48°34′43.77"E
5.	Xanegah	41°13′06.26"N	48°32′24.88"E
6.	Balbulaq	41°17'57.89"N	48°31'54.09"E
7.	Near villiage Püstegasim - Sample 1	41°16′09.47"N	48°35′21.81"E
8.	Near villiage Püstegasim - Sample 2	41°16′09.47"N	48°35′21.81"E
9.	Masalli Donuzuten	38°58'05.26"N	48°32'45.23"E
10.	Lerik Bülüdül Bulaq	38°39'17.02"N	48°36'59.47"E
11.	Lerik Haftoni Bulaq (Hovil villiage)	38°40'10.34"N	48°35'51.34"E
12.	Lerik Hamarmeshe Bulaq	38°44 <i>′</i> 33.57"N	48°36′33.37"E
13.	Lerik Aliabad Bulaq (Veri villiage)	38°50'22.33"N	48°26'36.60"E

Before the investigations, the thermal water samples were filtered and degassed slowly using the vacuum system. To stop vaporisation of pure water, the vacuum procedure was very slow (the groove of the flask valve, which held the sample, was very slightly opened).

The chemical compounds analysis (cations) were studied using a Spectroblue FMX 26 Optical Emission Spectrometer and DX 100 ion chromatography. Optical emission spectrometers with inductively coupled plasma (ICP plasma) as the excitation source offer ease of use, high sensitivity, precision and relative absence of interference. ICP-OES systems are now the analytical tool of choice for many applications. An ambient pressure density and speed of sound measurements at T = (278.15 to 343.15) K were measured using an Anton Paar DSA 5000 vibrating tube densimeter. The dynamic viscosity at T = (274.15 to 363.15) K were measured using an Anton Paar SVM 3000 Stabinger Viscometer.

THERMODYNAMIC FUNCTIONS OF FORMATION OF COMPOUND Cu₁₆Pb₂S₁₀

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The Cu-Pb-S system is of interest for metallurgy and semiconductor technology. The phase diagram of this system has been studied in detail. It is reported in the literature that the most stable compound is Cu₁₆Pb₂S₁₀, which is formed along the quasi-binary section PbS-Cu₂S at 752 K ÷ 790 K. Revealed only study [1], which gives the temperature dependence of the free energy of formation of Cu₁₆Pb₂S₁₀. However, it was revealed that the data given in [1] are not thermodynamic functions of the formation of the Cu₁₆Pb₂S₁₀ compound, but represent the sum of the heat capacity of simple substances: 16 mol of Cu, 2 mol of Pb and 10 mol of S. In this work, the thermodynamic functions of the formation of Cu₁₆Pb₂S₁₀ were determined by the method of electromotive forces (EMF). Measured EMF of concentration cells:

(-) $Cu_2S | Cu +, LiCl-KCl$ (eutectic mixture, 41.5 mol% KCl) | $(Cu_2S)_x$ (PbS)_{1-x} (+) (1) The potential generating process of the cells is:

$$Cu_2S + 1/4PbS \rightarrow 1/8Cu_{16}Pb_2S_{10}$$

(2) The choice of Cu₂S as a negative electrode is due to the fact that the electrode potentials of copper and lead differ little from aqueous solutions, melt of alkali metal chlorides, and the Cu₂S | Cu + electrode is more stable than the PbS Pb⁺² electrode and has a higher value of the electrode potential. Measurement of concentration chains (1) was carried out in the range 750 K \div 795 K for alloys with compositions x = 0.01 \div 0.96 mol fraction of Cu₂S. The results of measuring the EMF are shown in Table 1.

Table 1. EMF values of concentration cells (1)

T,K	E,mv	T,K	E,mv	T,K	E,mv
752	40.02	771	39,31	787	38,68
755	39,92	774	39,08	790	38,52
758	39,72	777	39,04	792	36.91
761	39,68	780	38,91	794	35.02
765	39,52	783	38,81	795	32.92
768	39,36	785	38,74		

For the temperature dependence of the emf of concentration cells (1), we obtained:

E,mv= (69,21163±0,58964) - (0,03884±7,63833E-4)T

Rounding off the coefficients of equation (3), we obtain:

E,mv= (69,2-38.8·10-3T

Based on the parameters of equations (3.4) and the well-known equations of thermodynamics for the partial molar Gibbs energy, enthalpy and entropy, we obtain:

$$\Delta \overline{G}_{760}^{0} = -7645 \pm 116 \text{ J/mol}; \ \Delta \overline{H}_{T}^{0} = -13356 \pm 500 \text{ J/mol}; \ \Delta \overline{S}_{T}^{0} = -7.49 \pm 0.4 \text{ J/(mol·K)}$$
 (5)

The molar thermodynamic functions of the formation of the $Cu_{16}Pb_2S_{10}$ compound are calculated by the equation:

$$\Delta Z_T^0 = \Delta \overline{Z}_T^0 + (1-x) \int_{x=0}^{x=0.04} \left[\Delta \overline{Z}_T^0 / (1-x)^2 \right] dx$$
(6)

Here: $\Delta \overline{Z}_T^0 \equiv \Delta \overline{G}_T^0$, $\Delta \overline{H}_T^0$, $\Delta \overline{S}_T^0$

In eq. (6) it was taken into account that in the range $x = 0.04 \div 0.80$ mol fraction Cu₂S, the EMF values are constant, do not depend on the composition, and in the range $x = 0.0 \div 0.04$ mol fraction Cu₂S_., they depend on the composition. The values obtained by equation (6) refer to the reaction:

$$Cu_2S+1/4PbS \rightarrow 1/8Cu_{16}Pb_2S_{10}$$

Then

$$8Cu_2S+2PbS \longrightarrow Cu_{16}Pb_2S_{10} \tag{7}$$

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(3)

(4)

Hence

$$\Delta Z_T^{0,*}(\operatorname{Cu}_{16}\operatorname{Pb}_2 \operatorname{S}_{10}) = 8 \,\Delta Z_T^0(\Delta \overline{G}_{360}^0, \,\Delta \overline{H}_T^0, \,\Delta \overline{S}_T^0)$$
(8)

Thermodynamic functions of formation of compound Cu₁₆Pb₂S₁₀ from Cu, Pb and S by reaction:

$$16Cu+2Pb+10S \rightarrow Cu_{16}Pb_2S_{10}$$
(9)

calculated by equation

 $\Delta Z_{T}^{0} (Cu_{16} Pb_{2} S_{10}) = \Delta Z_{T}^{0,*} (Cu_{16} Pb_{2} S_{10}) + 8 \Delta Z_{T}^{0} (Cu_{2} S) + 2 \Delta Z_{T}^{0} (PbS)$ (10)

The values of the thermodynamic parameters Cu_2S and PbS are taken from the source [2]. The results of the calculations are given in Table 2.

Table 2. Values of thermodynamic function s of the compound $Cu_{16}Pb_2S_{10}$ obtained from the elements, Cu_2S and PbS (* marked).

Compounds	$-\Delta C_{360}^0$	$-\Delta H_T^0$	ΔS_T^0	S_T^0	
	kJ/r	nol	J/(mol.K)		
Cu ₂ S(rhombic) [2]	94.5±1	77.5	22.4±1	120.9±2	
PbS(cubic) [2]	93.2±1	97.5±4	-5.6±1	91.2±2	
Cu ₁₆ Pb ₂ S ₁₀ (triclin)	862.5±4	941.7±15	-104.5±2	876.5±10	
*Cu ₁₆ Pb ₂ S ₁₀ (triclin)	61.2±1	106.8±5	-59.9±4	_	

In Table 2, the values of enthalpy and entropy of the compound $Cu_{16}Pb_2S_{10}$ belong to the range T = 752 ÷ 790 K. Since the difference in heat capacities of the compound and its components is very small, the values of $-\Delta H_T^0$ and ΔS_T^0 remain constant in the range T = 752 ÷ 790 K. In the source Cu₂S and PbS [2], the values given at room temperature were extrapolated to 760 K. A comparison of the enthalpy of formation of elements of the compound Cu₁₆Pb₂S₁₀ with the enthalpy of formation of this compound from Cu₂S and PbS shows that the energy

change per sulfide anion when three compounds are formed is about 10 kC / mol. This corresponds to the regu-

larity of enthalpy change when two-component chalcogenides are formed from two-component compounds.

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DETERMINATION OF THE BOUNDARIES OF IMMISCIBILITY OF THE LIQUID ALLOYS IN THE Cu-S SYSTEM

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Many studies have been carried out to determine the phase diagram of the Cu-S system [1]. However, there remains uncertainty about phase equilibria due to the strong tendency of the system to form several metastable phases. Compounds of the composition $Cu_{2-x}S$ and CuS are formed in various crystalline modifications. The most stable (up to 1130 C) is the face-centered cubic phase of stoichiometric composition Cu_2S . There are wide areas of immiscibility for liquid alloys. The fluid has two miscibility gaps: between L_1 and L_2 at temperatures above 1105 C in copper-rich formulations, and between L_2 and L_3 at temperatures above 813 C for a higher content of S. However, in the literature there are no reliable data on the immiscibility limit of liquid alloys in the Cu-S system. In this work, this problem is solved by thermodynamic calculations using some experimental data available in the literature. The calculation method described in [2] was used.

The calculation of the free energy of mixing liquid alloys is carried out according to the Gibbs-Helmholtz equation in the form:

$$\Delta G_T^0 = \Delta H - T\Delta S = [a + b(T - T_{mon.}) + c(P - P_{mon.})]x(1 - x) + RT[x \ln x + (1 - x)\ln(1 - x)]$$
(1)

In (1) the first term represents the enthalpy of mixing **AH** of liquid solutions in an asymmetric version of the model

of regular solutions; the second term represents the configurational entropy of mixing Δ S liquid solutions; *x*, *T*-mole fraction of the component, temperature for the immiscibility curve; T_{mon} , P_{mon} - temperature and pressure for monotectic reaction line; R= 8.314 J mol⁻¹ K⁻¹. For liquid solutions decomposing into two phases, the mixing parameter is a> 0; with increasing temperature and pressure, the immiscibility region narrows, therefore mixing parameter *b*<0 µ c<0; R= 8.314 J mol⁻¹ K⁻¹. To determine of the liquid immiscibility boundaries the thermodynamic condition of solutions of internal stability ($\partial^2 G/\partial x^2$)_{P,T}>0 was used [3].

To solve the equation (1) containing three functional parameters (composition, temperature, pressure) and Gibbs excess free energy, the Multipurpose Genetic Algorithm was used [2]. The following conditions were used to carry out the iteration process:

x=0÷1; a>0; b<0 ; c<0; T>T_{mon} ; P>P_{mon}

In particular, equation (1) for the immiscibility region of liquid alloys in the Cu-S system at $x_S = 0.4 \div 1$ was obtained in the form:

$$\Delta G_T^0(J/mol) = [30000 - 0.62(T - 1086) - 0.78P)]x(1 - x) + 8.314T[x \ln x + (1 - x) \ln(1 - x)]$$
(2)

Fig. 2 shows dependences of the free energy of mixing liquid Cu-S alloys on the composition at various temperatures and pressures For critical parameters of the considered immiscibility region of liquid alloys of the Cu-S system, the following data were obtained: T^{cr} =1883K (1610 C); P^{cr} =510 atm: $x_{\rm S}$ =0.7.

To determine the analytical dependences of the immiscibility boundaries on the composition, we used the calculated data for critical parameters and experimental data for the immiscibility coordinates shown in Fig. 1. In particular, the parameters of the analytical temperature dependence on the composition for the immiscibility curve in the Cu-S system at $x_S = 0.4 \div 1$ were obtained in the form

Value		
T,K	Intercept -2572,4	
T,K	B1	13034,6
T,K	B2	-9926,8
T,K	B3	555,6
Number of Points	7	
Degrees of Freedom	3	
Residual Sum of Squares	755,47619	
R-Square (COD)	0,99892	
Adj. R-Square	0,99783	

Consequently:

T,K= -2572,4+13034*x-9926,2*x^2+555,6*x^3, Here X=x_S

(3)

From (3) it follows that T^{kr} = 1883 K corresponds to the composition x_S = 0.7.



Figure 1. Phase diagram of the Cu-S system [1]. The boundaries of immiscibility of liquid alloys were determined in this work.

For the critical parameters of the regions of immiscibility of liquid alloys of the Cu-S system, we obtained: from the sulfur side: $t^{cr} = 1610 \text{ C} (1883 \text{ K})$ at $P^{cr} = 510 \text{ atm}$, $x_s = 0.7$ and from the copper side: $t^{cr} = 1810 \text{ C} (2083 \text{ K})$, $x_{Cu} = 0.85$. On the basis of these values, the boundaries of immiscibility of liquid alloys in the Cu-S system were determined (Fig. 1).

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GRAPHENE/PU/PMMA COMPOSITE FOR DESIGNING OF PROSTHESES: MOLECULAR ANALYSIS USING SEMIEMPIRICAL METHODS FOR DETERMINING THE EFFECT OF BLOOD FLOW ON COMPOSITE

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The field of nanoscience has increased in recent years in areas such as computing, sensors, biomedical and many other applications. Currently, nanomaterials have a huge variety of applications due to their structural characteristics; materials with improved physicochemical properties that are dimensionally more suitable in the field of nanoscience and technology are being examined [1]. In this regard, the discovery of graphene and graphenebased polymer nanocomposites is an important addition in the area of nanoscience, which plays a key role in modern science and technology. Graphene is considered a two-dimensional carbon nanofiller with a one atom thick flat sheet of sp2 bonded carbon atoms that are densely packed in a honeycomb-shaped crystal lattice, which has remarkable properties such as high thermal conductivity, superior mechanical properties and excellent electronic transport properties. The superior properties of graphene compared to polymers are also reflected in polymer/graphene composites showing better mechanical, thermal, and electrical properties compared to pure polymer. However, the improvement of the physicochemical properties of nanocomposites depends on the distribution of the graphene layers in the polymer matrix, as well as the interfacial bonding between the graphene layers and the polymer matrix. Interfacial bonding between graphene and the host polymer dictates the final properties of the graphene reinforced polymer nanocomposite [2], so that computational chemistry is an extremely useful tool since it allows to know and determine the behavior and interactions at the nanometric level through the calculation of molecular properties through the application of new computational technologies and mathematics to understand the systems at a chemical level. Currently the results obtained through computational chemistry have led it to be used in areas such as pharmacology, molecular biology, and organic and inorganic chemistry [3], for this it was used this tool to carry out this research consists of the development of a graphene-based nanocomposite for biomedical applications, specifically for the manufacture of prostheses, made using computational chemistry, made using computational chemistry, making use of simulated body fluid (SBF) which is a solution that contains concentrations of ions analogous to those of blood plasma, and allows predicting the bioactivity of some materials such as polymers [4].

KEYWORDS: Grafene, composite, prostheses

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THERMODYNAMIC CHARACTERISTICS OF COMPLEXING REACTIONS OF 2,2 , 3,4-TETRAHYDROXY-3 -SULFO-5 -NITROAZOBENZOLE WITH SOME METAL IONS

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Formaton of the same- and mixed-ligand complexes of pyrogallol-based azo compounds - 2,2', 3,4-tetrahydroxy-3'-sulfo-5'-nitrobenzene (R) with AI (III), Ga (III), In (III), Sn (II), Ti (IV), Zr (IV), Hf (IV), Mo (VI) and W (VI) ions have been studied. As a third component in the production of various mixed-ligand complexes cationic and nonionic surfactants as cetylpyridine bromide (SPBr), cetylpyridine chloride (SPCI), cetyltrimethylammonium bromide (STMABr), decamethoxine [1,10-decamethylene-bis (N, N-dimethylmentoxar) ammonium dichloride] (Dec), triton X-114; hydrophobic and hydrophilic amines - diphenylquanidine [1,2-diphenylquanidine] (DPhG), triphenylquanidine [1,2,3-triphenylguanidine] (TPhG), 1,10-phenanthroline (Phen), batophenanthroline [4,7-diphenyl-1, 10phenantholine] (Bphen) and ethylenediamine (ED) were used. AI (III), Ga (III), In (III), Sn (II), Ti (IV), Zr (IV), Hf (IV), Mo (VI) and W (VI) ions in acidic environment (pH 0-7.0) interact with reagent to form intensely colored same-ligand complex compounds. This is due to the fact that the reagent has a molecular form that is more suitable for complex formation reactions in acidic media [1]. In the presence of third components AI (III) -R-DPhG, Ga (III) -R-SPBr, Ga (III) -R-Triton X-114, In (III) -R-Triton X-114, Sn (II) - R-SPBr, Zr (IV) -R-TPhG, Hf (IV) -R-Bphen, Ti (IV) -R-Phen, Ti (IV) -R-Bphen, Mo (VI) -R-SPBr, Mo (VI) -R-SPCI, Mo (VI) -R-STMABr, Mo (VI) -R-ED, W (VI) -R-SPBr, W (VI) -R-SPCI, W (VI) -R -STMABr and W (VI) -R-Dec mixed-ligand complexes are formed. The formation of mixed-ligand complexes is often observed with the shift of the maximum yield to a more acidic environment (Table 1). This leads to the fact that mixed-ligand complexes have a higher stability than the corresponding to same-ligand complexes. The acidity interval (pHopt) corresponding to the maximum yield of the same- and mixedligand complexes formed by the reagent with metal ions was determined, and the effect of component concentration, time and temperature on the formation of the complex was studied.

The ratio of components in complex compounds was determined by various physicochemical methods. It was determined that the ratio of Me:R components in the composition of all same-ligand complexes is 1:2, in mixed-ligand complexes of AI (III) -R-DPhG, Ga (III) -R-SPBr, Sn (II) -R-SPBr, Zr (IV) -R -TPhG, Hf (IV) -R-Bphen, Ti (IV) -R-Phen, Ti (IV) -R-Bphen, Mo (VI) -R-SPBr, Mo (VI) -R-SPCI, Mo (VI) -R-STMABr, W (VI) -R-SPBr, W (VI) -R-SPCI, W (VI) -R-STMABr and W (VI) -R-Dec 1:2:2, in Ga (III) -R-Triton X-114, In (III) -R-Triton X-114 and Mo (VI) -R-ED 1:2:1. The stability constant of the studied complex compounds was determined by the spectrophotometric method, and it was found that the mixed-ligand complexes had a higher stability compared to the corresponding same-ligang complexes (Table 1).

Complex	pH _{opt}	lgβ	ΔG, kC/mol	Complex	pH _{opt}	lgβ	ΔG, kC/mol
Al(III)-R	3,6-4,0	6,21±0,04	-35,40	Ti(IV)-R	2,0-2,3	5,95±0,09	-33,92
AI(III)-R-DPhG	3,6-4,0	20,70±0,21	-117,99	Ti(IV)-R-Phen	2,5-3,0	14,82±0,14	-84,47
Ga(III)-R	2,0-2,3	8,12±0,05	-46,28	Ti(IV)-R-Bphen	1,0-1,5	16,19±0,17	-92,28
Ga(III)-R-SPBr	1,0-1,5	19,85±0,19	-113,15	Mo(VI)-R	1,8-2,0	8,67±0,14	-49,42
Ga(III)-R-Triton X-114	3,5-4,0	14,24±0,07	-81,17	Mo(VI)-R-SPBr	1,0-1,5	20,95±0,26	-119,42
Ga(III)-R-Phen	1,0-1,5	16,48±0,16	-93,94	Mo(VI)-R-SPCI	1,0-1,5	20,07±0,21	-114,40
İn(III)-R	4,0-4,4	5,64±0,09	-32,15	Mo(VI)-R-STMABr	1,8-2,9	19,45±0,24	-110,87
İn(III)-R-Triton X-114	3,0-3,5	13,02±0,09	-74,21	Mo(VI)-R-Dec	0,1-0,5 M H ₂ SO ₄	22,14±0,20	-126,20
Sn(II)-R	3,0-3,5	6,35±0,07	-31,20	Mo(VI)-R-ED	1,8-2,0	20,63±0,20	-117,59
Sn(II)-R-SPBr	0,5-1,0	17,75±0,21	-101,18	W(VI)-R	1,8-2,0	5,87±0,06	-33,46
Zr(IV)-R	2,0-2,3	6,52±0,08	-37,16	W(VI)-R-SPBr	1,0-1,5	17,05±0,20	-97,19

Table 1. Main characteristics of the same- and mixed-ligand complexes of 2,2', 3,4-tetrahydroxy-3'-sulfo-5'nitrobenzene.

Zr(IV)-R-TPhG	1,0-1,5	18,34±0,12	-104,54	W(VI)-R-SPCI	1,8-2,0	16,29±0,16	-92,85
Hf(IV)-R	2,0-2,3	7,19±0,11	-40,98	W(VI)-R-STMABr	1,8-2,0	16,01±0,18	-91,26
Hf(IV)-R-Bphen	0,5-1,0	14,17±0,17	-80,77	W(VI)-R-Dec	0,1-0,5 M H ₂ SO ₄	17,89±0,23	-101,97

The Gibbs free energy change of the formation of same- and mixed-ligand complexes of reagent with Al (III), Ga (III), In (III), Sn (II), Ti (IV), Zr (IV), Hf (IV), Mo (VI) and W (VI) ions was calculated using the equation $\Delta G = -R \cdot T \cdot InK$ [2]. All complex formation reactions were studied at room temperature: T = 298 K, R = 8.314 J/(mol·K). Since the equilibrium of complex formation reactions is characterized by a stability constant, the Gibbs free energy change of the formation reactions of the studied complex compounds was calculated using the equation $\Delta G = -5.70$ lg β (Table 1). The Gibbs free energy change (ΔG) of all complex formation reactions is characterized by a negative value. This suggests that the components of the same- and mixed-ligand complexes studied are formed by an exothermic reaction during the mixing of solutions, and that all reactions proceed spontaneously [3].

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POLYTHERMAL STUDY OF PHASE EQUILIBRIA AND SALTING OUT EFFECTS IN TERNARY SODIUM NITRATE + WATER + ALIPHALIC AMINES SYSTEMS

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Aliphatic amines and their aqueous solutions are widely used as industrial solvents. The dual systems waterdiisopropylamine and water-triethylamine are characterized by delamination with a lower critical solution temperature. Previously, the coordinates of the lower critical point of the water + diisopropylamine systems were clarified $(27.3^{\circ}C, 28.50 \text{ wt.\%} \text{ amine})[1]$ and water + triethylamine $(18.3^{\circ}C, 32.10 \text{ wt.\%})$ [2]. The water-dipropylamine system [3] has a lower critical point (- $4.7^{\circ}C, 27.2 \text{ wt.\%}$ amine) in the metastable region of the phase diagram. Our study is devoted to the study of phase equilibria in mixtures of components of triple systems sodium nitrate + water + diisopropylamine (- $17-90^{\circ}C$), sodium nitrate + water + dipropylamine (- $10-90^{\circ}C$), sodium nitrate + water + triethylamine (- $17-25^{\circ}C$) to determine the possibility of their use for the removal of amine from its aqueous solutions under the action of NaNO₃ and extractive crystallization of salt.

The study was carried out by the visual-polythermal method and the ratio of the volumes of liquid phases in mixtures of components of the specified systems. It is established that saturated and homogeneous solutions, monotectic and stratification are carried out in three-component mixtures. The analysis of the constructed phase diagrams of the systems at different temperatures allowed us to evaluate the effect of salting out amines from their aqueous solutions under the action of salt at different temperatures, as well as the efficiency of using amine in the process of extractive crystallization of NaNO₃.

To evaluate the efficiency of the process of salting out amines from aqueous solutions under the action of sodium nitrate, we determined the temperature dependence of the distribution coefficient K_d of the studied amines between the equilibrium liquid phases of the monotectic state. It was found that NaNO₃ has a large salting-out effect on mixtures of the binary water - diisopropylamine system. High values of the distribution coefficient of diisopropylamine (more than 550 in the range of 10-90°C), dipropylamine (more than 400 in the range of 10-90°C) and triethylamine (more than 100 in the range of 0-25°C) indicate that the salt is an effective salting agent of these amines. The concentration of amine in the organic phase reaches 88-96 wt.%, which is a favorable factor for the subsequent regeneration of amines after salt crystallization.

The effectiveness of the use of amines in the extractive crystallization of sodium nitrate was evaluated. It was found that the yield of NaNO₃ crystals in all the studied systems increases with an increase in the amine concentration in ternary mixtures. The peculiarity of the system with triethylamine was that with a maximum amine content of 90%, delamination in the system is observed only at 25°C and therefore the best salt yield (79.4%) was observed at this temperature. The maximum yield of sodium nitrate (~58%) for a system with diisopropylamine is realized at 0°C and 80.0 wt.% amine. With a slightly lower salt yield (54.8%) at 20°C, this temperature is more acceptable because it does not require cooling of the solution. In addition, the K_d at this temperature takes acceptable values (more than 900) for subsequent amine regeneration. In the ternary system with dipropylamine, the best salt yield was 78.2% with the introduction of 90 wt.% amine and 35.0°C.

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COMPARISON OF NRTL PARAMETER ESTIMATION STRATEGIES USING AN ARTIFICIAL NEURAL NETWORK FOR LIQUID-LIQUID AND VAPOR-LIQUID EQUILIBRIUM CALCULATIONS

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A numerical analysis on the NRTL parameter estimation procedure for several binary mixtures was performed. Multiple formulations using liquid-liquid (LLE) and vapor-liquid equilibrium (VLE) data were analyzed and compared in the parameter estimation problem including the application of an artificial neural network. Binary mixtures with both LLE and VLE regions were utilized. Simulated Annealing was used as the global optimization method in the thermodynamic data regression. The performance of NRTL model to describe the phase equilibrium behavior of both LLE and VLE using the binary interaction parameters obtained from tested formulations was assessed. Homogeneous and heterogeneous azeotropes were estimated using the different set of binary interaction parameters and results were used to complement the analysis of NRTL model performance. Results showed that the application of an artificial neural network in the parameter estimation process improved the model capabilities for the calculation of LLE. Regarding VLE calculations, some numerical challenges were found due to the presence of homogeneous and heterogenous azeotropes.

PECULIARITIES OF VAPORIZATION OF ALKYLIMIDAZOLIUM BASED IONIC LIQUIDS CONTAINING HIGH ELECTRONEGATIVITY ANIONS: A CASE OF [BMIM][BF4]

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Imidazolium based ionic liquids (ILs) due to their unique physicochemical properties are very attractive objects for industrial applications. Unlike common ILs having simple vapour composition consisting of neutral ion pairs (NIP), the ILs containing high electronegativity anions are characterized by the presence in vapour different decomposition products along with NIP. This phenomenon impedes the determination of vapour pressures and vaporization thermodynamics of such ILs. This work is devoted to investigation of vaporization of 1-butil,3-methylimidazolium tetrafluoroborate [BMIM][BF₄] by complex approach including Knudsen effusion mass spectrometry, gas phase chromatography - mass spectrometry, NMR and IR spectroscopy, thermal analysis and quantum-chemical calculations.

A serial sector magnetic mass spectrometer equipped by molybdenum Knudsen cell (vaporization to effusion area ratio of ~400) was used to study of IL under study (Sigma-Aldrich, 99.9%). Gaseous species were ionized by the electrons with energy of 40 eV and emission current of 0.25 mA. Thermal analysis of the samples was performed on a synchronous thermal analysis instrument Netzsch STA 449 F3 Jupiter in the temperature range 20-500 °C at a speed of 5 K/min in nitrogen atmosphere.

Among studied possible processes of IL vaporization (Fig. 1) three competing routes of $[BMIM][BF_4]$ congruent evaporation have been revealed: in the form of NIP; in the form of BMImBF₃ and HF; in the form of 1-methylimidazole, 1-butene, HF and BF₃. Two other possible routes of dissociative evaporation of $[BMIM][BF_4]$ in the form of bicyclic IL and H₂ as well as 1-butylimidazole, H₃CF and BF₃ are found to be negligible.

The [BMIM][BF₄] vapor composition is strongly affected by three key factors (in the order of decrease): the ratio of the surface area of sample to its volume, temperature, and time. In equilibrium conditions (Knudsen cell) imidazole-2-ylidene dominates in vapor, otherwise in Langmuir conditions (open surface) the evaporation in the form of NIP is preferred. A decrease of the NIP amount in vapor was also observed upon heating (approximately 4 times from 450 K till 510 K). IR spectroscopic measurements were carried out on a Bruker Tensor 27 spectrometer with Fourier transform. NMR spectra ¹H, ¹³C, ¹¹B, ¹⁵N in DMSO-d6 at T = 22 °C and T = 70 °C were recorded by a Bruker Avance 500 spectrometer with 5 mm TBI 1H/31P/D-BB z-GRD sensor. The GCMS experiments were carried out on a Shimadzu GCMS QP2010 Ultra.



Figure 1. Schemes of [BMIM][BF₄] decomposition

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COMPARATIVE STUDY OF INFLUENCE OF ETHANOL AND 2,2,2-TRIFLUOROETHANOL ON THERMOPHYSICAL PROPERTIES OF 1-ETHYL-3-METHYLIMIDAZOLIUM DICYANAMIDE IN BINARY MIXTURES: EXPERIMENTAL AND MD SIMULATIONS

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This work focuses on studies of influence on several thermophysical properties of ionic liquid (IL), 1-ethyl-3methylimidazolum dicyanamide ([EMIM][DCA]) by alcoholic solvents, ethanol, and 2,2,2-trifluoroethanol (TFE) experimentally and computationally. Herein, the densities, ρ , speeds of sounds, u, and dynamic viscosities, η , of pure IL, [EMIM][DCA], molecular solvents; ethanol and TFE and their binary mixtures have been measured over the entire mole fraction ranges and at various temperatures from 298.15 to 323.15 K, with an interval of 5 K and at pressure P = 0.1 MPa. The obtained experimental data are utilized to determine the excess/deviation properties viz. the excess molar volumes, V^{E} , isentropic compressibility deviations, ΔK_{s} and viscosity deviations, $\Delta \eta$. The excess/deviation properties of the studied binary mixtures are fitted to polynomial equations of the Redlich-Kister type. The dependence of computed parameters on composition and temperature and the nature of studied systems are discussed in terms of ion-ion, ion-dipole, hydrogen bonding and dipole-dipole interactions. The excess molar volumes of each binary system have been correlated with the Prigogine-Flory-Patterson (PFP) theory. To get a molecular-level understanding of the interactions between the IL and co-solvent, Molecular Dynamics (MD) Simulations is employed for two different systems as a function of composition at two different temperatures. Along with thermophysical properties such as density and excess molar volume, the self-diffusion coefficient, radial distribution function (RDF), and coordination number are also obtained from MD to provide further insight fluorine substituted ethanol (TFE) with IL in order to understand the effect of substitution of fluorine in ethanol in the IL + solvent binary and ternary systems.

KEYWORDS: Thermophysical properties, Molecular Dynamic Simulations, 1-ethyl-3-methlimidazolium dicyanamide ([EMIM][DCA]), 2,2,2-trifluoroethanol (TFE), ethanol, Molecular dynamics simulations.



NUMERICAL CHARACTERIZATION OF PHASE STABILITY PROBLEMS USING STOCHASTIC GLOBAL OPTIMIZATION METHODS: A PROPOSAL FOR A RELIABLE SET OF REFERENCE PROBLEMS

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In Chemical Engineering, the optimization plays an important role in solving different problems including thermodynamic calculations such as phase stability analysis and equilibrium modeling. Phase stability analysis is a fundamental stage in phase equilibrium calculations in multicomponent and multiphase systems. This analysis is used to characterize the thermodynamic behavior of a mixture in terms of phases and compositions that it will present under given operating conditions. The phase stability problem can be solved by minimizing the tangent plane distance function (TPDF). Different TPDF problems have been used in literature to evaluate and compare the performance of optimization techniques. However, the characteristics and numerical complexity of these phase stability problems have not been evaluated and it is unknown if these systems really correspond to global optimization problems suitable to evaluate and compare available stochastic global optimization methods (SGO). This work is a first approach to propose a set of phase stability reference problems to evaluate and identify the advantages and limitations of SGO techniques. This study has focused on the characterization and classification of a set of phase stability problems according to their resolution complexity via the evaluation and analysis of several metrics associated with the performance of different SGO methods. A subset of problems with appropriate characteristics, including TPDF problems from low to high resolution complexity, is proposed to allow a reliable comparison and evaluation of current and new SGO methods. The results of this study highlight the relevance of developing and improving SGO methods to reliably perform phase stability analysis.

PHASE TRANSITION HEAT STORAGE ENERGY EFFICIENCY EVALUATION BASED ON MELTING TERMOGRAM

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In developing heat storages (HS) on the basis of phase transitions (PhT) the main efforts are now focused on developing the HS form, calculating various features of design and such parameters of phase transition heat storage material (PhT HSM) as volume, HS surface area, heat transfer coefficient (or thermal resistance) on the border of HSM with HS, temperature and charging and discharging time, energy efficiency. At the same time, the physical problem of taking into account the processes of the phase transitions themselves and their influence on the effective operation of the HSs is poorly covered.

In this paper, on the basis of our own extensive experience in the experimental study of melting and crystallization processes and their theoretical description, we give some recommendations for taking into account the peculiarities of phase transitions when analyzing the effectiveness of PhT HSM. The options for charging (Ch) and discharging (D) of HS based on PhT HSM are considered in accordance with the heating and cooling thermograms for two cases: during melting and quasi-equilibrium crystallization (QEC), as well as during melting and non-equilibrium-explosive crystallization (NEC) [1].



Figure 1. Thermograms of melting and QEC (a) and NEC (b).

The amount of heat accumulated by HSM when heated is

$$Q_A^Z = m_A \left[\int_{T_1}^{T_L} c_S(T) dT + \Delta H_{LS} + \int_{T_L}^{T_2} c_L(T) dT \right], \qquad (1)$$

where m_A – HSM mass, c_S , c_L – the specific heat capacities of HSM in the regions of the solid and liquid phases respectively in the temperature ranges from T_1 up to T_L and from T_L up to T_2 ; T_1 and T_2 are HSM temperatures at the beginning and at the end of charging, ΔH_{LS} and T_L are melting enthalpy and melting point of HSM.

The amount of heat obtained by the HS during the period of discharge without taking into account the heat losses during the QEC (Fig. 1, a) is determined by the expression

$$Q_A^R = m_A \left[\int_{T_L}^{T_2} c_L(T) dT + \Delta H_{SL} + \int_{T_1}^{T_L} c_S(T) dT \right], \qquad (2)$$

where ΔH_{SL} – crystallization enthalpy; in case of QEC ΔH_{SL} = ΔH_{LS} .

The total heat released during discharge in the case of NEC is equal to

$$Q_A^R = m_A \left[\int_{T_L}^{T_2} c_L(T) dT + \left(\Delta H_N + \Delta H_C + \Delta H_{cr}^{'} \right) + \int_{T_1}^{T_L} c_S(T) dT \right],$$
(3)

where ΔH_N , ΔH_C , $\Delta H'_{cr}$ – enthalpies of nucleation, coagulation of nuclei, and crystallization [1].

Total enthalpy of non-equilibrium crystallization is equal to

$$\Delta H_{SL} = \Delta H_N + \Delta H_C + \Delta H'_{cr} \,. \tag{4}$$

Depending on the values ΔH_{LS} , ΔH_{SL} , ΔH_{N} , ΔH_{c} , $\Delta H'_{cr}$, as well as the corresponding periods of time for each type and stage of crystallization, the efficiency of PhT HS can vary significantly:

$$\eta_{A} = \frac{Q^{R} - Q_{0}^{R}}{Q^{Z} + Q_{0}^{Z}},$$
(5)

where Q^{Z} is the heat of charging HS; Q_{0}^{Z} – heat loss during charging; Q^{R} – heat of discharge HS; Q_{0}^{R} – heat loss during discharge.

So when developing HS on the basis of HSM PhT, it is proposed to take into account the thermophysical features of crystallization of various HSMs by thermographing and calculating the energy efficiency of the process.

KEYWORDS: heat storage material, phase transition, thermogram, melting, crystallization, efficiency, energy efficiency.

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KINETICS OF THE DEPOSITION OF COPPER IONS ON MARBLE IN THE PRESENCE OF A COMPLEXING AGENT

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Currently, low-grade and off-balance sheet deposits are becoming increasingly important in the mining and metallurgical industries. They are characterized by refractory and refractory ores with a low metal content. The best enrichment technologies to date make it possible to extract metal with its content in the ore of the order of 0.2-0.3%. With further development of the deposit, ores with a copper content of 0.1-0.2% and less remain undeveloped. Also, a significant amount of copper is found in the dumps of copper mines and tailing dumps. Thus, the development of methods for additional recovery of non-ferrous metals from poor and off-balance ores and dumps is an important and urgent task in connection with the constant reduction of mineral reserves in rich deposits.

Our earlier calculations showed that the formation reactions of malachite and azurite with the participation of organic ligands are thermodynamically probable [1]. In the case of lactic acid, as the temperature rises, the change in the Gibbs energy increases, and the reverse reaction becomes more preferable. Authors [2] used this circumstance in their work, where lactic acid was used to dissolve copper from malachite ore at temperatures up to 70 °C.

The aim of this research was to study the kinetic aspects of the deposition of copper ions on marble from a solution of copper lactate with the formation of malachite. The process under study is of practical importance for the development of methods for extracting off-balance metal in deposits and dumps of spent copper.

The results obtained show the possibility of using environmentally friendly organic complexing agents to increase the geochemical migration of copper ions. According to kinetic measurements, the release of malachite from copper lactate complexes on calcite is relatively high. A growing layer of oxidized carbonate copper minerals is gradually formed on carbonate materials, which can subsequently be processed by known beneficiation methods.

Based on the experimental data obtained on the rate constants, it is possible to estimate the growth rate of basic copper carbonates when interacting with organic complexing agents. In accordance with the obtained reaction rate constants, the growth time of a 1 mm thick sediment layer is of the order of 400-500 days in the case of copper lactate. As a result, the concentration of copper in carbonate materials increases compared to the original rocks, copper losses in dumps are reduced and environmental safety is increased.

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EXPERIMENTAL STUDY OF THE NONISOTHERMIC AND NONLINEAR FILTRATION USING THE LAYERED MODELS FOR EASTERN SIBERIA DEPOSITS

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Effect of the nonisothermic process of filtration on the filtration-capacitive and production parameters of reservoir have been studied within the framework of the two-dimensional non-stationary filtration model for the hydrocarbon mixture at the thermobaric conditions of the Eastern Siberia Deposits. The porous core and a multicomponent hydrocarbon mixture typical for the oil and gas fields of Eastern Siberia as a reservoir model were chosen.

In the course of laboratory studies of core and fluid samples the data of the filtration-capacitance and thermophysical parameters of MP characteristic of oil and gas for Eastern Siberia deposits have been obtained using the author's experimental methods. These made it possible to most accurately calculate the distributions of pressure and temperature fields taking into account the nonlinear law of the reservoir fluid flow, to investigate an effect of the non-isothermal filtration process on the reservoir component recovery and to determine the areas of dynamic condensation in MP taking into account nonlinear non-isothermal filtration. In this case, a change in the temperature of the filtered mixture in the core entails phase transformations of the mixture at a pressure corresponding to the beginning of condensation, which is different from the pressure of the beginning of condensation process and, therefore, changes the value of the component transfer and saturation with the phases of the core.

The novelty of the approach lies in the synthesis of theoretical and experimental studies, namely, that due to the use of experimental data on thermophysical and filtration-capacitance parameters directly in the system of nonlinear differential filtration equations, it becomes possible to accurately predict changes in the phase behavior of hydrocarbons in the reservoir and the features of their filtration flows for given thermophysical parameters of the mixture and core.

KEYWORDS: hydrocarbon mixture, nonstationary and nonisothermic filtration, phase transitions, thermobaric conditions.

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OBTAINING OF HIGH QUALITY DIESEL FUEL FROM HYDROCRACKING PROCESS OF VACUUM GAZOIL

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Increasing the depth of oil refining and improving the quality of exported oil products with the involvement of heavier and higher sulfur oils remains one of the key problems in the oil refining industry. Hydrocracking of heavy oil raw materials meets the specified requirements of the oil refining industry, and this leads to an increase in the strength of the hydrocracking process. Among hydrocracking processes, because of their high quality and demand, the processes aimed at obtaining kerosene and diesel fractions as the main product are of the more interest. Hydrocracking processes differ in both reagent delivery and the raw material flow, as well as process conditions and characteristics of the used catalysts according to these conditions. For example, only hydrogen sulfide-resistant catalysts can be used in a single-stage hydrocracking process, for reusable applications, it is important to use catalysts that reformed bulk polynaphthene molecules, especially polycyclic condensed aromatic compounds, as, otherwise, these compounds will accumulate in the recirculating residue, which can lead to decreased conversion, reduced catalyst life, and even plant failure [1]. In order to remove undesirable impurities during any variant of hydrocracking, the raw material is first passed through the catalysts of the protective layer, then underwent to hydrofining and only then to hydrocracking.

In presented thesis, the aim of done work was to obtain environmentally friendly diesel fuel and high-quality raw materials for catalytic cracking process by hydrocracking of vacuum gas-oil obtained from Baku oils in the presence of modified aluminosilicate catalyst containing Ni, Mo.

The hydrocracking process of vacuum gas-oil conducted at 3-8 MPa pressure, 400-460 °C temperature range, in a flow-type Hungarian unit with a reactor capacity of 200 ml. The liquid product obtained from the process distillated to gasoline (o.p.-200°C), diesel fraction (200-360 °C) and residue > 360 °C in an atmospheric vacuum unit. Each fraction studied separately.

The effect of regime parameters on hydrocracking process of vacuum gas-oil was studied. The influence of pressure on hydrocracking process of vacuum gasoil, conducted in the presence of alumosilicate catalysts modified with Ni and Mo, was investigated. The effect of pressure on hydrocracking process was studied at the range of 3-8 MPa. Based on the results of the effect of pressure on the hydrocracking process of vacuum gas oil, it was determined that when the pressure increases from 3 MPa to 5 MPa, the yield of the diesel fraction increases from 35% to 44% weight. The output of diesel fraction growths to 48 % with further increasing of pressure from 5 MPa to 8 MPa. That is, only 4% increase is observed. It was considered expedient to carry out the hydrocracking process at 5 MPa, as icreasing the pressure from 5 MPa to 8 MPa leads to a relative increase in capital costs.

Thus, the possibility of obtaining of 44-48% weight of diesel fraction and also, raw material for catalytic cracking process from hydrocracking of vacuum gas oil (obtained from Baku oil mixture) carried out in the presence of aluminosilicate catalyst modified with Ni, Mo metals was shown.

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DENSITY OF IONIC LIQUIDS AT HIGH PRESSURES AND WIDE RANGE OF TEMPERATURES

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lonic liquids (ILs) are ideal solvents for green chemistry, have various positive properties (negligible vapor pressure, non-flammable, low melting point, high solvating capacity, low compressibility, high ionic conductivity etc.), which make them attractive for practical applications. In order for design and developing reliable predictive models and to understand the nature of molecular interactions in liquid mixtures and to decide whether the IIs are suitable as a part of novel working pair, the basic thermodynamic properties (density, viscosity, heat capacity, compressibility, thermal expansion coefficient etc.) are required.

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-ethyl-3-methylimidazolium trifluoromethanesulfonate [EMIM][TFO] and 3-methyl-1-pentylimidazolium tetrafluoroborate [C₅MIM][BF₄] at pressures up to p = 140 MPa and wide T = (273.15 to 413.15) K range of temperature. The temperature in the measuring cell was measured with an expanded absolute uncertainty of U(T) = 0.015 K. Pressure was measured using a pressure transmitters P-10, P-30 (0.25, 2.5, 50, 100 MPa) and new HP-2 (160 MPa) with an expanded relative standard uncertainties U of (p,ρ,T) measurements in: U(p) = 0.00025 MPa for p < 0.25 MPa, U(p) = 0.0025 MPa for p < 2.5 MPa, U(p) = 0.01 MPa for p < 10 MPa, U(p) = 0.1 MPa for p < 100 MPa. The observed repeatability of the density measurements, also attending the high viscosity corrections to vibration tube periods, have an expanded uncertainty within $\Delta p/\rho = \pm(0.01 \text{ to } 0.08)\%$.

The ambient pressure density $\rho(p_0, T)$ values were measured using Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibrating tube densimeters with an uncertainty in $\Delta \rho = \pm (5 \cdot 10^{-3} \text{ to } 3 \cdot 10^{-1}) \text{ kg} \cdot \text{m}^{-3}$. The heat capacities $c_p(p_0, T)$ of ILs at ambient pressure and various temperatures were measured using the Pyris 1 and µDSC 7 Evo differensial scanning calorimeters DSC.

An empiric equation of state for fitting of the (p, ρ, T) data has been developed as a function of pressure, temperature and molecular mass of [EMIM][TFO] and [C₅MIM][BF₄] ILs. This equation together with the heat capacity values was used for the calculation of the thermophysical properties of these ILs, such as isothermal compressibility $\kappa_T(p,T)/MPa^{-1}$, isobaric thermal expansibility $\alpha_p(p,T)/K^{-1}$, thermal pressure coefficient $\gamma(p,T)/MPa\cdotK^{-1}$, internal pressure $p_{int}(p,T)/MPa$, specific heat capacities $c_p(p,T)/J\cdotkg^{-1}\cdotK^{-1}$ and $c_v(p,T)/J\cdotkg^{-1}\cdot K^{-1}$, speed of sound $u(p,T)/m\cdots^{-1}$, isentropic expansibilities $\kappa_s(p,T)$ at high pressures and temperatures, in which the density of ILs were measured. The available literature values of these ILs were compared with obtained in this work values.

THE ENERGY AND EXERGY INVESTIGATIONS OF THE DEEP EUTECTIC SOLVENTS IN ABSORPTION REFRIGERATION CYCLES

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In the last recent years, more studies were carried out about absorption refrigeration cycles due to their energy saving advantages. In absorption refrigeration cycles, the compression section which is the main unit in the conventional vapor-compression cycles is replaced by an absorber and regenerator unit. Accordingly, an appropriate absorbent with special characteristics is required to be used in absorption refrigeration cycles. In this work, a feasibility study for using of three common-used Deep Eutectic Solvents, DESs (Reline, Ethaline, and Glyceline) which are very recent introduced green solvents, as absorbent in absorption refrigeration cycles were investigated. Also, ammonia was considered as refrigerant. The vapor liquid equilibria calculations by using gamma-phi approach were used for determining the thermodynamic properties of DES/ammonia working pair. According to the investigated cycles were determined. Also, exergy analyses as a powerful tool for investigating the less and most exergy destructive sections of the investigated cycles was carried out.

KEYWORDS: Refrigeration, Deep Eutectic Solvents, green solvent, absorption, Energy, Exergy.

CARBON DIOXIDE SOLUBILITY IN IONIC LIQUIDS

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lonic liquids (ILs) are regarded as environmentally-benign solvents due to their immeasurably low vapor pressure. Recently, significant progress has been made in the application of ILs as alternative solvents for carbon dioxide (CO_2) capture due to their broad range of liquid temperatures, excellent thermal, chemical stabilities and other physical and chemical properties. Due to the high solubility of CO_2 in ILs, they can be used for the extraction of various gases from gas mixtures

In this work, we present the high pressure CO₂ solubility measurements in ILs 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [EMIM][NTf₂], 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [BMIM][NTf₂], 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [IMIM][NTf₂] and 1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide [OMIM][NTf₂] at [T=(273.15 to 413.15) K, p=(0.101 to 5) MPa] together full literature analysis. The high pressure CO₂ solubility measurements were carried out using the constructed isochoric method with an experimental uncertainty of $\Delta m = \pm 0.0005$ mol·kg⁻¹ in CO₂ solubility. The installation uses the full automatic LabView Software control system and consists of three main parts: a) gas reservoir, b) stainless steel measuring (equilibrium) cell, c) electronic control system box. The stabilization of the temperature in the measuring cell is controlled using the external thermostat (Kälte-Umwälzthermostat LAUDA ECO RE 415 Gold, Germany) with an error of ±10 mK using the (ITS-90) PT100 thermometer, which is connected to the thermostat via PT-100 Libus Modul. The pressure transducers (PAA33X-V-100, Omega Engineering inc., 0-100 bar, Newport Electronics GmbH, Germany) were used for the definition of pressure.

The obtained solubility values in ILs were fitted to the polynomial equations using the molality or mole fraction of CO_2 . The fugacity coefficient of CO_2 and Henry's law for the solubility was calculated using the fugacity *f* of CO_2 .

INVESTIGATION OF HYDROCRACKING PROCESS OF FUEL OIL IN THE PRESENCE OF MODIFIED HALLOYSITE

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One of the most important problems of oil refining industry is to deepen oil refining by involving heavy oil residues to the treatment. One of the main processes used for the changingof heavy oil residues (fuel oil, goudron) into gasoline, diesel and other light products is cracking process. The hydrocracking process of fuel oil conducted at 0,5-4,0MPa and 400-450°C, in the presence of halloysite and halloysite modified with Mo, Ni by impregnation and ion-exchange methods in CVD (Chemical Vapor Deposition) unit was investigated [1].

The influence of temperature on hydrocracking process of fuel oil in the presence of Mo+Ni/halloysite was studied at 1,0MPa pressure and 400-450 °C temperature range, but effect of pressure at 440 °C and 0,5-4,0 MPa pressure range. When temperature rises from 400 °C to 440 °C the yield of light oil products increases from 28,25 to 64,56% wt. Meantime the yield of gas, gasoline and diesel fractions increases from 4,91 to 9,45%; from 8,25 to 31,02%; from 20 to 33,54% wt., respectively, the amount of coke also rises from 1,63 to 4,73% wt. With increasing of temperature from 440 °C to 450 °C the yield of light oil products lessens from 64,56 to 56,12%, the amount of gas increases from 4,73 to 8,1%, this is explained by the deepening of the cracking process.

With increasing of temperature from 430 °C to 450 °C in composition of gasoline fraction the amount of iso-paraffins increases from 41,45 to 51,09%, the yield of olefins reduces from 8 to 4,98% and the octane number constitutes 73 p. The amount of sulphur decreases from 0,08 to 0,04% wt., iodine number from 16,3 to 7,3 gJ₂/100g in composition of gasoline. The content of resin, amount of sulphur and iodine number are decrease in composition of diesel fraction. The results of effect of pressure on hydrocracking process of fuel oil in the presence of halloysite modified by Mo and Ni by ion-exchange method. When the pressure rises from 0,5 MPa to 4,0MPa the yield of Σ fr.<360°C fraction increases from 59,3 to 66%, the amount of coke lessens from 4 to 2%.

The change of pressure also influence on qualitative indicators of obtained products. With increasing of pressure from 0,5 MPa to 4,0 MPa in composition of gasoline fraction the yield of aromatic and unsaturated hydrocarbons decreases from 7 to 3,5% and from 6,02 to 2,11%, respectively, the amount of iso-paraffins increases from 41 to 45%, the yield of sulphur reduces from 0,075 to 0,0421 %wt., the octane number of gasoline constitutes 76p.

Thus, from the studies of hydrocracking process of fuel oil in the presence of natural zeolites and modified catalysts it can concluded that, when process is conducted at low pressure (0,5 MPa) the yield of gasoline fraction is higher, but in relatively high pressures (4,0MPa) the yield of diesel fraction is higher. Depending on purpose, it is possible to achieve high yield of desirable product by changing of pressure and temperature.

The possibility to obtain extra light oil products and to increase the oil refining depthwas shown as a result of hydrocracking process of fuel oil in the presence of natural zeolites and their nanostructured with transition metals forms. Gasoline and diesel fractions obtained from hydrocracking process of fuel oil after hydrorefining process can be used as components for commercial grade fuels, gasoline fraction also can be used as raw material for pyrolysis, obtained gas can be used as fuel in Refinery and residual fraction can be used for bitumen production.

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THERMODYNAMIC FUNCTIONS OF THE CuGa2InTe5 COMPOUND

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A study of the nature of phase formation in the In₂Te₃-Cu₂Ga₄Te₇ system at a 1:1 ratio of the initial components revealed a new CuGa₂InTe₅ compound congruently melting at 1128 K. In [1], the thermophysical properties of this compound were studied and a mixed mechanism of charge carrier scattering and heat transfer was established, associated with the multicomponent composition and complexity of the band structure. This paper presents the results of calculations of the thermodynamic functions of CuGa₂InTe₅.

The heat of atomization of the compound was calculated. It was determined that $H_S(CuGa_2lnTe_5)=213.017$ kJ/mol. Then, using the thermodynamic data of individual elements that make up the quaternary compound $CuGa_2lnTe_5$ [2, 3], the standard heat capacity, entropy, enthalpy, and free energy of formation were calculated. To calculate the heat capacity, the Neumann-Kopp method was used [3]: $C_p(CuGa_2lnTe_5)=205.79$ J/(mol·K).

Knowing the melting point of the compound under study, as well as the melting and Debye temperatures of the individual elements included in the composition, one can use the Debye method to calculate the characteristic Debye temperature, and then, using the Magnus-Lindemann equation, the isochoric heat capacity [4].

The entropy of the CuGa₂InTe₅ compound was determined by Kelly method [3] and it was found that $\sum S_{298}^{0}$ (CuGa₂InTe₅) =1591.466 J/(mol·K). Using the values of the isobaric heat capacity, the standard entropy can be calculated. Therefore, S_{298}^{0} (CuGa₂InTe₅) =279,13 J/(mol·K). The entropy of formation of the CuGa₂InTe₅ compound is calculated as the difference between the standard entropy and the entropy of the constituent simple substances. Since the CuGa₂InTe₅ compound is formed with an open maximum when the ratio of the initial components is 1:1, then ΔS_{298}^{0} = -1312.336 J/(mol·K). Calculations of the enthalpy of formation of the CuGa₂InTe₅ compound have shown that ΔH_{298}^{0} (CuGa₂InTe₅) =-708.76 kJ/mol.

The standard free energy of formation was calculated using the Gibbs-Helmholtz equation [5]. It was determined that ΔG_{298}^0 =-317.684 kJ/mol. The negative value of the standard energy of formation indicates the stability of the CuGa₂InTe₅ phase.

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MODELLING OF THERMOPHYSICAL PROPERTIES OF MOLTEN FLUIDS FOR HEAT TRANSFER APPLICATIONS

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Molten salts (fluoride, chloride, and nitrate) are used as heat transfer fluids as well as for thermal storage in molten salt power plant such as concentrated solar plants and molten salt reactor. Operating temperature of this system is very high. After research work done till 1970s it was found that molten fluoride salts are stable at high temperatures, have good heat transfer properties and can dissolve high concentration of actinides and fission products.

Accurate data of thermo physical property is required there is large discrepancy of available data. Experimentation for obtaining data of thermo physical properties is hard and complex at high temperature. With advent of computers modeling thermophysical properties of multicomponent system can overcome most of these difficulties.

The aim of this paper is to predict properties like density, viscosity and thermal conductivity because these are important properties required for heat transfer and storage. Ternary fluoride salt have low melting point therefore using Generic Solution Model and Unit cell model properties will be studied .GSM model proposed by Chou was used to study density and viscosity and has been demonstrated to work with reasonable accuracy. Thermal conductivity was studied using unit cell model. These values were also compared with other models available from literature. The results of the current model were found to be more reasonable theoretically, reliable in practical application and more realistic to use in computerized thermodynamic and phase diagram calculation.

KEYWORDS: Molten salt, Fluoride salt, Geometric Modeling, Unit cell model, Density, Viscosity, thermal conductivity.

EXERGETIC ANALYSIS OF A MATERIAL AND ENERGY RECOVERY FROM MUNICIPAL SOLID WASTES IN HAVANA

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In Havana there is no segregated collection of municipal solid wastes (MSW) at the origin, being landfills are the main final disposal method of MSW. Material Recovery Facility (MRF), is the preferred method for treating the recycling stream. In MRF, in addition to recyclable materials, refuse-derived fuel (RDF) is obtained, which is sent to the Energy Recovery Facility (ERF) (i.e., incineration and gasification) to generate electricity. Exergy analysis is a quantitative assessment of solid waste treatment systems in the industrial ecology perspective. The exergy concept contributes to a better assessment of the sustainability of technology concerning resource management. The exergetic analysis allows evaluating the thermodynamic imperfections (i.e., irreversibilities) of a process quantitatively. In this work, the exergetic analysis of an MRF plant integrated into an ERF for the adequate treatment of Havana's MSW was carried out. The mass, energy and exergy balances of the MRF and ERF were performed in Excel and the process simulator Aspen Plus v.10.0, respectively. The gravimetric composition was varied (±10%) to see the effect on the global exergetic efficiency of the MRF plant and each area of the ERFs analyzed. For this, three groups were accounted: biodegradable waste (BW) (79.4%), plastics (8.3%), and others (i.e., metals and glass; 12.3%). By reducing (-10%) the BW (71.4%), the global exergy efficiency of the MRF increases from 53.9% (base case) to 56.6%. If the BW increases by 10%, the global exergetic efficiency decreases to 51.4%, while if only the plastic fraction increases by 10%, the global exergetic efficiency increases to 54.2%. By increasing the BW and plastic fraction simultaneously, the global exergetic efficiency decreased to 51.7%.

In the RDF incineration process, the combustion chamber turned out to be the area with the lowest exergetic efficiency (40.5%), leading to ~75% of the total exergy destruction. In this ERF (i.e., incineration) the pumps had the lowest exergetic destruction, 0.04% with respect to the total exergetic destruction. In incineration, in the base case, the air temperature is 25 °C and an excess of 100% input in the combustion chamber, by increasing the air excess to 300% the exergetic efficiency decreases to 31.2% (-23 %) because the combustion chamber temperature decreases and if the air temperature is increased to 100 °C, the exergetic efficiency increases to 43.7% (+ 8%). In the RDF gasification process, the gasifier turned out to be the area with the lowest exergetic efficiency (44.2%), leading to ~71% of the total exergy destruction. In this ERF (i.e., gasification) the syngas cooling had the lowest exergetic destruction, 1.7% with respect to the total exergetic destruction. In the gasifier, an increase in the air ratio to 0.4 decreases the exergetic efficiency to 29.6% (-33%). The total exergetic destruction of the incineration process is slightly higher (1.32%) than that of gasification. The exergetic destruction of the combustion chamber in the incineration process is higher (8.2%) than that of the gasifier, which shows that the gasification process is more exergetically efficient than the incineration process. This work allows to know the areas of the greatest exergy destruction in the thermochemical treatments of RDF, as well as the operating variables that must be controlled to obtain greater exergetic efficiencies. This is beneficial for the more exergetically efficient design of waste to energy plants.

KEYWORDS: Municipal Solid Waste, Material Recovery Facility, Refuse Derived Fuel, Energy Recovery Facility, Exergetic efficiency

SYNTHESIS OF N-ALKYL BROMINE-SUBSTITUTED IONIC-LIQUID MONOMER AND POLYMER BASED ON IT

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The problem of protecting the environment one of the global problems confront humanity in the twenty-first century. In this respect creating new, environmentally efficient production and chemical processing technologies is one of the most promising direction in chemical industry. In this aspect the synthesis of ionic-liquid monomers and polymers and copolymers based on them with high molecular weight and a new set of properties are in the focus of researchers' attention as a promising direction in the chemistry of high molecular weight compounds [1].

This thesis presents the results of studies carried out at the Institute of Petrochemical Processes of ANAS on the synthesis of an ionic liquid monomer-N, N-diethyl-N- (2-bromethyl) -N- (2-methacryloxyethyl).) ammonium bromide, as well as its polymerization. The synthesis of the indicated bromine-containing ionic liquid monomer was carried out in two stages. In the first stage, 1,2-dibromoethane reacts with the amine component - diethylaminoethanol, in the appropriate molar ratio taken. The compound obtained in a yield of 96% - N, N-diethyl-N- (2bromethyl) -N- (2-hydroxyethyl) -ammonium bromide in the second stage reacts with methacryloyl chloride, synthesized in turn by a known method [2].

Obtained in 98% yield ionic liquid salt - N, N-diethyl-N- (2-bromethyl) -N- (2-methacryloxyethyl) ammonium bromide. The structure of the synthesized monomers was studied by IR and ¹H NMR spectroscopy. The elemental composition of the monomer determined on a PERKIN ELMER-2400 device showed almost complete corresponding between the obtained data and the calculated ones. The melting point (87-89 °C) and the ionic conductivity of the sample were determined, and at various concentrations of aqueous (0.1; 0.3; 0.5 and 1.0%; wt.) solutions and with an increase in the concentration of the solution, a slight increase (2.3·10⁻³; 2.7·10⁻³; 2.9·10⁻³; 3.1·10⁻³ (S·cm⁻¹)) in ionic conductivity of synthesized ionic liquid monomer was observed.

The process of polymerization of the synthesized monomer was carried out in an aqueous medium in the presence of the initiator azobisisobutyronitrile (AIBN). Various factors influencing the polymerization process have been studied: temperature, amount of initiator, concentration of monomer in aqueous solution, polymerization time, and conditions have been established that ensure a high yield of polymer based on ionic-liquid monomer. These types of polymers are suitable for use as electrically conductive and absorbent materials.

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IONIC LIQUID IN THE PROCESS OF EXTRACTION OF PETROLEUM FRACTIONS OF VARIOUS PURPOSES

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Despite the versatility of the fields of application of ionic liquids, it is of particular interest to use them as a selective solvent in the process of extraction refining of oil fractions. Since by varying the cation and anion of the ionic liquid, a solvent can be obtained that has a set of unique properties characteristic of the extractant.

The presented thesis reflects the results of the extraction purification of a hydrotreated diesel fraction, as well as an AMG-10 hydraulic fluid with an N-methylpyrrolidone acetate ionic liquid. The content of aromatic and sulfur compounds in the composition of the diesel distillate was 16 wt% and 311 ppm, respectively, and the content of aromatic compounds in the composition of the hydraulic fluid distillate was 14 wt%.

By studying various factors on the process of extraction purification of the indicated oil fractions, the dependence of the degree of dearomatization on the conditions of purification was established. In particular, on the basis of the studies carried out, it was found that during the extraction purification of diesel distillate, the optimal condition for obtaining an almost completely dearomatized fuel is a two-fold weight excess of the ionic liquid to the raw material, the contact time of the components is 1 hour and room temperature (20-25 °C). It should be noted that, in this case, the content of sulfur compounds in the composition of refined diesel fuel decreases 2,4 times and is 130 ppm.

In the case of selective purification of the distillate of the AMG-10 hydraulic fluid using an ionic liquid of the indicated composition, almost complete dearomatization of the distillate under study is also achieved at a temperature of 60 °C, a contact time of 2 hours and a weight ratio of raw material: extractant - 1: 2,5.

Comparison of the results of extraction purification of two petroleum distillates with different purpose shows that to obtain AMG-10 hydraulic fluid with practically zero content of undesirable components, in particular aromatic hydrocarbons, the AMG-10 distillate extraction process must be carried out under relatively harsh conditions as compared to diesel distillate extraction. factions. This is apparently due to the relatively high viscosity of the AMG-10 hydraulic fluid. Thus, the kinematic viscosity of the AMG-10 distillate used as a raw material is 2,13 mm²/s (at 50 °C) versus 3,40 mm²/s (at 40 °C) of diesel distillate.

From the presented material, it follows that the ionic liquid - N-methylpyrrolidone acetate is promising for the selective purification of oil fractions for various purposes with the selection of conditions optimal for this raw material.

SYNTHESIS OF A NEW Al_2O_3-B_2O_3 BASED CATALYST FOR OLIGOMERIZATION OF OLEFINS

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In recent years, the use of large alken fractions obtained during oil refining in the synthesis of high-octane components for fuels by catalytic refining is considered one of the most promising ways. Given a number of advantages of heterogeneous processes in comparison to homogeneous (easy separation of the catalyst from the reaction products, return of the catalyst to the system and the absence of wastewater generated during the process, etc.), researchers are focusing on the development of environmentally friendly heterogeneous processes in oligomerization of alkenes. Zeolite-based catalysts, which are widely used in the oligomerization of olefins, are strongly decontaminated due to their coating with high-molecular compounds formed during the reaction. For this reason, much researches are currently focused on the creation of new heterogeneous catalytic systems that are characterized by maximum activity, selectivity, and stability. For this purpose, some works were carried out to prepare a gamma-Al₂O₃ catalyst modified with boric oxide in different proportions. Using the sol-gel method in the preparation of the catalyst, Al(NO₃)₃·9H₂O underwent to hydrolysis process in the presence of monoethanolamine at room temperature, first Al(OH)₃ sol is obtained and then by raising the temperature to 80-90°C its gel was obtained [1-3]. The obtained gel was washed several times with distilled water and dried, then mixed with orthoboric acid solution in different proportions and thermal treated.

The obtained product was determined by scanning calorimetric method. The results of thermogravimetric analysis of the H₃BO₃-Al(OH)₃ system revealed the interaction of the components with increasing temperature. Based on the DTG/DTA results, it can be said that the separation of physically adsorbed and crystallized water in the samples (dried at 120°C) is accompanied by endothermic peaks in the temperature range of 150-200°C. The peaks in the DTG and DTA curves in the temperature range of 300-500°C are associated with the production and crystallization of y-alumina as a result of dehydration of Al(OH)₃ [4]. An increase in the amount of boric oxide in the samples by up to 20% is accompanied by an expansion and a decrease in the intensity of the galon in the thermogram. In addition, the presence of exo-effect in the temperature range of 700-850°C in the DTA curves of the samples and the loss of mass in the DTG-curve can be explained by the formation of a crystalline structure containing $2AI_2O_3 B_2O_3$. With the increase of B_2O_3 in the system by the RFA method, a decrease in the size of the crystallite during heat treatment at the same temperature was determined, which is fully consistent with the DTA/DTG results of the samples. It was found that modification of nano y-aluminum oxide (1-20% by weight) with boric oxide in quantities allows to obtain nanomaterials with a developed surface (S_{special surface}=190-280 m²/g, V_{pore}= 0.43-0.60 cm³/g). Oligomerization of the decene-1 conducted in the temperature range of 150-200°C for 1-5 hours in the presence of the synthesized catalytic system Al₂O₃-B₂O₃, the optimal conditions for the process were selected. It was found that the catalyst shows stable activity in the oligomerization process, is characterized by high thermal resistance, which increases the usability of the catalyst by returning it to the system several times.

KEYWORDS: Heterogeneous catalyst, sol-gel method, metal oxides, thermogravimetric analysis

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ABOUT THE OLIGOMERIZATION OF HEXENE-1 IN THE PRESENCE OF AN ALUMINUM-BASED CATALYTIC COMPLEX MODIFIED WITH CHROMIUM SALT

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The application of high-quality lubricants in machines and engines is one of the important factors for efficient and environmentally friendly operation. Because of its low freezing point, high thermostability, resistance to oxidation, coking and homogeneity, polyalphaolefin (PAO) oils have always been in the focus of researchers.

Taking into account a number of shortcomings of cation-type catalysts traditionally used for oligomerization processes (high hygroscopicity, multi-stage preparation process, instability), we conducted research on the synthesis of new catalytic systems with high activity and stability. For this purpose, catalytic systems — CTC (was synthesized from aluminum and 1,2-dichloroethane) and its modification with chromium salt — CTC/CrCl₃ were synthesized for oligomerization and alkylation processes, the structures of these systems studied by physical methods, the process of oligomerization of hexene-1 with their participation was comparatively studied, the possible mechanism of the process is given. It was found that in the presence of a new catalytic complex modified with chromium salt, it is possible to obtain oligomers with high yield and physical performance, characterized by a narrow molecular weight distribution during the oligomerization of hexene-1 [1-2].

Thermooxidation stability of oil fraction (fr.300-500°C) obtained from oligomerization of hexene-1 in the presence of CTC and CTC/CrCl₃ was studied by the method of differential scanning kalorimeters (DSK), based on the results of the analysis it was determined that polyalphaolefin oils obtained in the presence of CTC/CrCl₃ are more resistant to temperature effects than those obtained in the presence of CTC: the maximum decomposition temperature was recorded at 285°C when CTC was taken for oligomerization of hexene-1, in the CTC/CrCl₃ system this value changed to 330°C, the resulting difference was 45°C. Oligohexene fraction analyzed by ultraviolet (UV) spectroscopic method, intensive absorption bands (195-200 nm) of double-bonded unsaturated hydrocarbons practically very weakly observed, signals related to aromatic hydrocarbons (260-280 nm) is not registered. The absence of aromatic hydrocarbons and unsaturated hydrocarbons in the obtained oils opens up prospects for their use as "White oil" in medicine, even without the use of hydrogenation. The study of oil fractions obtained in the CTC/CrCl₃ system by the method of nuclear magnetic resonance (¹³C NMR) revealed that the synthesized oil fractions do not contain carbon atoms belonging to olefin structures, at the same time, the formation of weak signals characteristic of naphthenic rings in the sample is noteworthy. This fact confirms the oligomerization properties of the used bimetallic catalytic system, as well as the fact that it directs the products obtained during the process to cycling - naphthenic ring compounds.

Polyalphaolefin oils obtained from oligomerization of hexene-1 with the participation of new catalytic systems differ from base oils in terms of high viscosity. It was found that from the oligomerization of hexene-1 in the presence of CTC/CrCl₃ it is possible to obtain oils with the 89% yield, high viscosity index (120-135), low freezing point (-45÷-48°C), with a narrow molecular weight distribution (M_w/M_n =1.12-1.16) and these oils can be recommended for use as high quality engine oils.

KEYWORDS: catalytic complex, oligomerization, hexene-1, polyalphaolefin

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THERMODYNAMIC PROPERTIES OF SOME RARE EARTH METALS TELLURIDES

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Rare earth elements (REE) chalcogenides with high thermal stability and unique magnetic, optical, and thermoelectric properties are among the promising functional materials [1, 2]. Development and optimization of methods for directed synthesis of new phases are based on data on phase equilibria in the corresponding systems and thermodynamic properties of intermediate phases [3]. Even though the phase diagrams of most binary systems of the Ln-Te type have been studied in detail [4], the thermodynamic properties of REE tellurides are practically not studied. There is an estimated date on the enthalpy of formation and entropy of a number of compounds of the Ln_2Te_3 and LnTe types [5,6].

This work summarizes the data on the thermodynamic properties of some lanthanide tellurides (Ln-Nd, Gd, Tb, Er, Tm, Yb), obtained by us by the method of electromotive forces (EMF). For the thermodynamic investigations of the intermediate phases of the above state systems, the following concentration cells were assembled

(-) Ln (s.) | glycerol + KCl + LnCl₃ | (Ln in alloys) (s.) (+) (1)

(-) LnTe (s.) | glycerol + KCl + LnCl₃ | (Ln in alloys) (s.) (+) (2)

and their EMF were measured in the 300-450 K temperature range.

Cells of type (1) were used to determine the partial molar functions of Ln in monotellurides, and cells of type (2) were used to determine the partial properties of LnTe in alloys richer in tellurium. The detailed descriptions of the methods for the preparation of the electrodes and electrolyte and assembly of the electrochemical cell were described in [7-9].

LnTe and alloys – anodes of the cells of type (1) and (2) were synthesized by the ceramic method by melting of elementary components of high purity in evacuated (10⁻²Pa) graphitized silica ampoules at 1000K. The phase compositions of the alloys were controlled by powder X-ray diffraction analysis (PXRD). By combining the experimental data of the obtained concentration chains of types (1) and (2), the partial thermodynamic functions of Ln in the alloys are determined, based on which the standard thermodynamic formation functions and the standard entropies of the intermediate compounds are calculated. A comparative analysis of the obtained data with the literature is carried out.

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THERMODYNAMIC PARAMETERS of Ga_{0.5}In_{1.5}Se₃ at HIGH TEMPERATURE

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Chalcogenide semiconductors are widely used compounds. It is known that the physicochemical properties of these compounds are related to their crystal structure. Therefore, it is important to study the crystal structure of these compounds. With cation-cation substitution in chalcogenides, many processes in the crystal structure can be observed: phase transitions, structural transformations, phase formation. Chalcogenides of the A_2B_3 type are one of the most widely studied semiconductor compounds. It was found that the thermal properties of these compounds depend on the ionic radii of the A and B atoms. The crystal structures of these compounds have been studied for a long time. However, the effect of cation-cationic substitutions on the crystal structure and thermal properties in these compounds has not been studied. In this work, the compound $Ga_{0.5}In_{1.5}Se_3$ was synthesized, its crystal structure and thematic properties were studied. The values of thermodynamic parameters were determined by analyzing the DSC spectra obtained in the temperature range 25 °C $\leq T \leq$ 950 °C.

The synthesis process was carried out according to the standard procedure. The thermal properties of the object under study were carried out by the method of differential scanning calorimetric analysis (DSC). DSC was performed on a Jupiter STA 449F3 (Netzsch, Germany). The analysis was carried out in a dynamic mode in an inert atmosphere (helium) on a thermal analyzer at a heating rate of 5 deg/min, using a Pt-Pt/Rh thermocouple. The device operates under the control of "Proteus" software. The experiments were carried out in the temperature range T = 25-950 °C.

The physical characteristics of the heat flow characterize the structural processes , the degradation mechanism and important processes such as oxidation in the compounds. The transition from the heat flux function to the heat capacity and the temperature values of the heat capacity make it possible to explain the mechanism of change in thermodynamic functions. In the compound Ga_{0.5}In_{1.5}Se₃ the heat flux rate $\Delta \Phi$ curve was obtained at a constant heat treatment rate of 5 °C/min. The temperature dependence of the heat flux was characterized by two main effects. The powdery nature of the Ca_{0.5}In_{1.5}Se₃ sample creates a weak mechanism of interaction with water molecules entering the diffusion region on the surface of nanoscale crystals.

The central peaks of the described effects correspond to temperatures $T_1 = 102$ °C and $T_2 = 848$ °C. The central peak at 102 °C in the temperature range $25 \le T \le 455$ °C in the DSC spectrum of the Ga_{0.5}In_{1.5}Se₃ compound shows the characteristics of the decomposition of water molecules falling into the diffusion region onto the crystal surface. For this effect, it was determined that the value of the heat flux function increases to 0.23 µV/mg and goes into a stable region at a temperature of 455 °C. It was also determined that the energy of the field generated by the thermal function is 7.54 mJ, and the entolpy value is 1.35 J/gThe thermodynamic parameters of the effect with a central peak at $T_2 = 848$ °C in the temperature range $778 \le T \le 850$ °C of the Ca0.5In1.5Se3 compound are also calculated. It was determined that the value of the heat flux function changed to 0.01 µV/mg, the energy of this area of influence was 0.68 mJ, and the enthalpy was 0.0021 J/g.

THERMOPHYSICAL CHARACTERIZATION OF THE OXALINE MIXTURE

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INTRODUCTION Natural Deep Eutectic Solvents (NADESs) [1] have been proposed as an alternative to traditional solvents due to their biodegradability and biocompatibility [2]. They are prepared by mixing two or more compounds of natural origin at moderate heating thus the procedure is cheap, easy, and 100% efficient. All of these characteristics are essential principles of 'green chemistry'.

EXPERIMENTAL The NADES studied here is formed by choline chloride as H-bond acceptor and oxalic acid as H-bond donor in the mole ratio 1:1. In the literature, sometimes is called oxaline and it was obtained from Scionix, Ltd.

RESULTS We present experimental data of several thermophysical properties of oxaline in the temperature range of (278.15 - 338.15) K and at atmospheric pressure. They were densities, speed of sounds, refractive indices, isobaric molar heat capacities, surface tensions, kinematic viscosities, and electric conductivities. The thermodynamic properties (density, speed of sound, refractive index, isobaric molar heat capacity and surface tension) were linearly correlated (1) with the temperature and the transport properties (dynamic viscosity and electric cal conductivity) were exponentially fitted with the Vogel-Fulcher-Tammann expression (2): $Y = A \cdot T + B$ (1)

$Y = Y_0 \cdot \exp\left[B / (T - T_0)\right]$						
Table 1. Fitting parameters and their corresponding root-mean square relative deviations, <i>RMSD</i> _r .						
Property	А		В	RMSD _r (%)		
r / (g·cm⁻³)	-0.000701	1	.43984	0.01		
<i>u</i> / (m·s⁻¹)	-2.370	2	582.67	0.06		
n _D	-0.0002725	1.	544046	0.00		
s / (mN·m⁻¹)	-0.0474		86.22	0.03		
C _{p,m} / (J·mol ⁻¹ ·K ⁻¹)	0.4367		208.18	0.06		
Property	h_0	В	T_0	RMSD _r (%)		
<i>h</i> / (mPa⋅s)	0.09988	859.385	181.02	1.14		
Property	k_{∞}	В	$\overline{T_0}$	RMSDr (%)		
<i>k</i> / (mS·cm ⁻¹)	1204.2	-568.7	197.99	1.33		

CONCLUSIONS

In this contribution, a comprehensive thermophysical characterization, in a wide temperature range and at atmospheric pressure, of the NADES containing choline chloride and oxalic acid in (1:1) molar ratio is presented. These results will contribute to the implementation of this eco-friendly solvent in different industrial processes.

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CLUSTER-ASSOCIATE MODEL OF THE VISCOSITY OF THE LITHIUM CARBONATE

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The authors of the monograph [1] have developed a model for determining the regularity of viscosity by temperature based on the concept of chaotic particles, which does not contradict, but even complements the classical theory of viscosity. According to this concept, developers rely on the virtual presence of liquid and gaseous phases in the solid state of a substance. The cluster-associate model of the viscosity of a liquid makes it possible to estimate the degree of association of clusters or their number based on the temperature dependence of the viscosity. The accepted concept is expressed by the formula:

$$\eta = \eta_1 (T_1/T)^{a = a_2(T_2/T)^b}, \tag{1}$$

where η_1 – is the reference experimental (reference) point of dynamic viscosity at temperature T_1 (K); a – is the degree of cluster association; b – is the degree of aggregation of cluster associations.

The lithium carbonate data were taken from the reference book [2] and the following were selected as reference values from the presented values: $T_m = 891$ K, $T_1 = 1050$ K, $\eta_1 = 4,64$ mPa·s, $T_2 = 1080$ K, $\eta_2 = 3,67$ mPa·s, $T_3 = 1120$ K, $\eta_3 = 2,83$ mPa·s. The necessary values were calculated: $a_2 = 8,3250$; $a_3 = 7,6611$; b = 2,2851. Then a_2 and b were substituted into the expression (1)

$$\eta = 4,64 (1050/T)^{8,3250(1080/T)^{2,2851}}.$$
(2)

The calculation results for all viscosity values are shown in Table 1.

Table 1. Reference [2] and dynamic viscosity data calculated by the formula (2) for lithium carbonate

Т, К	<i>η</i> [2], mPa·s	η (2), mPa·s	а
<i>T_m</i> = 891	-	38,72	12,92
1050	4,64	4,64	8,88
1060	4,34	4,27	8,69
1070	4,01	3,95	8,5
1080	3,67	3,67	8,33
1090	3,36	3,42	8,15
1100	3,1	3,2	7,98
1110	2,91	3,01	7,82
1120	2,83	2,83	7,66

The correlation coefficient when comparing the reference data [2] with the proposed cluster-associate model (2) of viscosity is quite high R = 0,994364 and $t_R = 4,98 >> 2$, which indicates the adequacy of the new dependence.

The cluster-associated viscosity model made it possible to construct a model for lithium carbonate. According to the available reference data, the high adequacy of the presented cluster-associate model of the dynamic viscosity of lithium carbonate has been established.

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NEW PHASES OF VARIABLE COMPOSITION IN THE MnTe–Ga₂Te₃–In₂Te₃ SYSTEM

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Complex chalcogenides of transition metals, in particular, compounds of the AB₂X₄ type (A-Mn, Fe, B-Ga, In, Sb, Bi, X-S, Se, Te) are important functional materials with magnetic, optical, photoelectric, thermoelectric, topological, and other properties [1-4]. By changing the composition of these compounds to obtain solid solutions of various types of substitution, their functional characteristics can be significantly improved. Taking into account the above, the purpose of this work was to study phase equilibria in MnTe-Ga₂Te₃-In₂Te₃ (A) system.

For investigations, first, the binary compounds of system A in evacuated to $\sim 10^{-2}$ Pa, and sealed quartz ampoules were synthesized. Samples of the studied system were prepared by fusion of the synthesized compounds also under vacuum conditions. To achieve complete homogenization after melting, all alloys were thermally annealed at 800 K for 500 hours and cooled in a switched-off furnace. Some alloys, after being kept at the indicated temperature, were quenched by dropping ampoules into cold water.

DTA was performed on the simultaneous thermal analyzer Netzsch STA449 F3 (platinum-platinum-rhodium thermocouples). Phase and structural studies were carried out based on powder diffraction data obtained on a D2 Phaser diffractometer (CuK α 1 radiation) using the Eva and Topas 4.2 programs.

Based on the analysis of experimental data obtained, the projection of the liquidus surface, as well as a number of polythermal and isothermal sections of the phase diagram of the system (A), were constructed. In Fig. the diagram of solid-phase equilibria at 800 K is shown. As can be seen, the system is characterized by the formation of regions of solid solutions of various lengths based on the compounds Ga₂Te₃ and In₂Te₃ (β -phase), MnIn₂Te₄ (γ ₂-), MnGa₂Te₄ (γ ₁-),



and (α -). It should be especially noted that the homogeneity region of continuous solid solutions of the Ga₂Te₃-In₂Te₃ boundary system significantly (25–30 mol%) penetrates deep into the concentration triangle and occupies a significant part of its area (β area). The revealed new phases of variable composition are of interest as magnetic materials.

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ELECTRICAL PROPERTIES OF Cd_{1-x}Mn_xSe THIN FILMS

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 $Cd_{1-x}Mn_xSe$ semimagnetic semiconductors (SMSC) are the focus of intense research of scientists due to their unique properties combining of magnetic and semiconducting properties. They are employed in a variety of devices including solar cells, gas sensors etc. Thin films of $Cd_{1-x}Mn_xSe$ SMSC are some advantages on their bulk crystals. In this work we investigate electrical conductivity of $Cd_{1-x}Mn_xSe$ ($0 \le x \le 0.1$) thin films, defined the activation energies depending on temperature and Mn concentration.

Cd_{1-x}Mn_xSe ($0 \le x \le 0.1$) thin epitaxial films were successfully prepared using Molecular Beam Condensation (MBC) method in a vacuum of $(1\div 2)10^{-4}$ Pa on a glass substrates. The different thin film obtaining parameters such as temperature, time of evaporation, speed, etc. were optimized to yield good quality samples. The substrate temperature was $T_{sub} = (640 \div 670)$ K and source temperature was $T_{sub} = (1100 \div 1200)$ K. Epitaxial films was growing in the (111) plane of a face-centered cubic lattice.

The structure and phase purity of the Cd_{1-x}Mn_xSe ($0 \le x \le 0.1$) epitaxial films were checked at room temperature by means of X-ray powder diffraction (XRD) using a BRUKER XRD D8 ADVANCE. The electrical conductivities were measured in the temperature range T= 300 K ÷ 500 K. It was defined that the conductivity increased with temperature and the activation energies. It was observed that the room temperature electrical conductivity increased with the composition parameter $x \le 0.1$. The increase in the electrical conductivity is obviously due to the decrease in the band gap and enhanced grain structure of the material. In our previous works we defined that band gap of the Cd_{1-x}Mn_xSe ($0 \le x \le 0.1$) thin epitaxial films decrease with increase of Mn content. The high temperature region is characterized by a grain boundary-limited conduction mechanism and the low temperature zone by a hopping conduction mechanism.

The thermoelectric voltage was found to be negative in all films, indicating n-type conduction in the samples. Thus, the thermoelectric power measurements of $Cd_{1-x}Mn_xSe$ ($0 \le x \le 0.1$) epitaxial films showed n-type conduction. It is also observed that the temperature variation of thermoelectric power is approximately linear at low temperature, but exhibits non-linear behavior at higher temperatures, obeying the power law dependence of temperature.

KEYWORDS: Semimagnetic semiconductor, thin film, XRD, conductivity, activation energy.

GROWTH PROPERTIES OF Cd_{1-x}Mn_xS SOLID SOLUTION THIN FILMS

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One of the important issues in material science is to obtain a new semiconductor materials, research of their physical properties, purposeful management and identification of application opportunities in instrumentation engineering. In recent decades, semimagnetic semiconductors (SMSC) have become the subject of extensive research. SMSC are alloys with magnetic ions diluted in nonmagnetic semiconductors. The presence of magnetic elements in these semiconductors allow to obtain structures on their base managing by magnetic field.

 $Cd_{1-x}Mn_xS$ SMSC are new semiconductor materials belonging to the group of A^{II}B^{VI} type semiconductors. The epitaxial films of these SMSC are considered to be of special importance for fundamental research and practical application.

Few works in the literature have been devoted to the study of their physical properties. In the present work we report a preliminary study on the synthesis of $Cd_{1-x}Mn_xS$ (x=0.05, 0.1) solid solutions and preparation of perfect epitaxial films on their base.

 $Cd_{1-x}Mn_xS$ solid solutions were synthesized in a vacuumized quartz ampoules by impurity of primary components - Mn and CdS semiconductor compounds (purity not less than 99.99). Synthesized $Cd_{1-x}Mn_xS$ (x=0.05 and 0.1) solid solutions were used to grow epitaxial films.

The preparation of $Cd_{1-x}Mn_xS$ (x=0.05, 0.1) thin films on glass substrates was carried out using the molecular beam condensation method in a vacuum of $(1\div 2)10^{-4}$ Pa. Thin films of polycrystalline structure were grown on glass substrates at temperature 470 K and source temperature 1100 K.

The structural properties of the prepared films were studied by X-ray diffraction measurements on a Bruker D8 Advance XRD. The XRD patterns of $Cd_{1-x}Mn_xS$ thin films at various Mn concentrations (x=0, 0.05, and 0.1) display an intense diffraction peak at approximately (26.6°) which coincides with the [002]/[111] diffraction line of the (CdS) hexagonal/cubic crystalline phase. The film with *x*=0 shows high degree of crystallinity and as manganese ion concentration increases, the degree of crystallinity gradually decreases (the peaks have a large width) due to quantum confinement.

KEYWORDS: Semimagnetic semiconductor, synthesis, thin film, X-ray diffraction measurement, lattice constant, polycrystalline.

OBTAINING ACTIVE ALUMINIUM OXIDE – A SUPPORT FOR HYDROPROCESSING CATA-LYSTS IN OIL REFINING

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The most common support for hydroprocessing catalysts in oil refining is active aluminium oxide (AAO) that plays not only a role of an inert diluent and also participates in formation of active phases, serves as an active structural promoter creating a specific porous structure that is optimal for processing of a specific feedstock [1].

Methods for preparation of AAO and its modification for obtaining a support with required structural and textural properties are an important part of catalyst synthesis technology. The porous structure of AAO consists of micro-, meso- and macropores [2]. Micropores are parasitic formations. The metals of active phases, trapped in the micropores become inaccessible to molecules of feedstock, i.e. inactive. Macro- and mesopores are of the same nature and gapes or cavities between aluminium oxide crystals. Macropores are transport pores through which feedstock molecules penetrate in the volume of catalyst granule and as a result, catalytic processes can occur not only on the outer surface of the granule. Macropores have a large total volume and a small surface. The main working pores of the catalyst are mesopores, in which the vast majority of catalytic acts occur. Mesopores have large volumes and surfaces. Mesoporous aluminium oxides are most commonly produced by evaporation-induced self-assembly using a soft or hard template. In accordance with this method, a solution is prepared containing an aluminium oxide precursor and a surfactant (SAS) dissolved in water or another solvent. Subsequent evaporation of the solvent leads to the formation of an orderly organized mesoporous inorganic material. The properties of the final mesoporous product significantly depend on the initial ratio of surfactant/aluminium oxide precursor [3].

Recently, the syntheses have been carried out in IPCP on modifications of alumosilicate catalyst transition metals (Ni, Co, Mo) by impregnation method and hydropurification process of vacuum gasoil obtained from Azerbaijani petroleums mixture, gasoline, light and heavy gasoil obtained via coking process, light gasoil mixture obtained via catalytic cracking has been performed in the presence of them. Desulfurization rate has amounted to 90-93%. The investigations are continued in this direction.

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COMPARISON OF THE THERMAL CONDUCTIVITY DATA BETWEEN A THW AND A TLS SENSOR

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When considering measuring the thermal conductivity of liquids, the two most popular methods referred to in the literature are Transient Line Source (TLS) and Transient Hot Wire (THW). The Transient line source is constructed in needle form and designed for testing soil and solid materials (ASTM D5334, IEEE442-2017). Test times range from 30 to 90 second depending on length of sensor, with typical total temperature rise from transient in the range of 5 to 10 °C.

Transient Hot-Wire technique is in wire form and is designed following a full theory for testing liquids (ASTM 7896-19). The measurement time is 1 second, with typical total temperature rise from transient in the range of 2 to 4 °C. When testing solids with TLS, there is no concern in the effects of convection. When testing liquids, the constant applied power and the high temperature rise can result in the presence of convection and significant errors in results.

Measurements with THW have been optimized to better control the convection. Different applied powers depending on the measured liquid, the short measurement time, and the low temperature rise, minimize the effect of convection and increase the results accuracy.

As observed, from the experimental data, on the TLS measurements there is an increasing uncertainty trend based with decreasing viscosity due to the longer test times of the TLS method and the presence of convection. This effect is amplified when testing the thermal conductivity with temperature.

SOLID PHASE EQUILIBRIA IN THE GeTe-SnTe-Bi2Te3 SYSTEM

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Ternary tetradymite-like compounds formed in the A^{IV}-B^V-Te systems (A^{IV}-Ge, Sn, Pb; B^V-Sb, Bi) are perspective thermoelectric materials [1]. Recent studies have shown that these compounds also exhibit topological insulator properties and can be used in spintronics, quantum computing, terahertz detectors, etc. [2,3]. One of the ways to obtain new multicomponent phases and materials based on known ones is to study phase equilibria in systems composed of compounds-structural or formula analogs.

This paper presents the results phase equilibria investigations in the GeTe-SnTe-Bi₂Te₃ quasi-ternary system (A). The boundary quasi-binary components GeTe-Bi₂Te₃ and SnTe-Bi₂Te₃ of this system are characterized by the formation of a number of analogous compounds, in particular, with the A^{IV}Bi₂Te₄, A^{IV}Bi₄Te₇, and A^{IV}Bi₆Te₁₀ compositions. This allows us to expect the formation of wide regions of substitutional solid solutions in the system (A). The synthesis of compounds and alloys of the system (A) was carried out by fusing high-purity elementary components in evacuated (~ 10⁻² Pa) quartz ampoules. After alloying, the samples were quenched from 1000 K into cold water and then annealed at 600 K for 1000 h.

The studies were carried out by DTA (NETZSCH 404 F1 Pegasus system), XRD (Bruker D8 diffractometer, CuK_{α}- radiation), and SEM (PhilipsXL-30 FEG). Based on the obtained experimental results, the diagram of solid-phase equilibria of system (A) was plotted (Fig.). It was found that the system is characterized by the formation of continuous series of solid solutions along the GeBi₂Te₄-SnBi₂Te₄, GeBi₄Te₇-SnBi₄Te₇, and GeBi₆Te₁₀-SnBi₆Te₁₀ sections. The parameters of the crystal lattices of the obtained phases with variable composition are determined by the indication of the powder diffraction patterns. The system also revealed wide regions of homogeneity based on the GeTe, SnTe, and Bi₂Te₃ compounds. The obtained new phases are of great interest as potential termoelectric materials and topolgical insulators.



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VISCOMETRIC PROPERTIES OF BINARY MIXTURES CONTAINING 1,4-BUTANEDIOL AT DIFFERENT TEMPERATURES

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The viscosities of binary mixtures of 1,4-butanediol with 2-methoxy ethanol and 2-propoxy ethanol have been determined at 303.15, 308.15, 313.15 and 318.15 K over the entire mole fraction range. The deviation in viscosity, $\Delta\eta$, and excess Gibbs energy of activation (ΔG^{*E}) of viscous flow have been examined in terms of structural changes and interactions. The deviations/excess values fitted to the Redlich-Kister equation to determine the fitting parameters and the root-mean square deviations. The results obtained for viscosity of binary mixtures were used to test the semi-empirical relations of Bingham, Frenkel, Kendall, Hind Ubbelhode, Refutas, Sutherland Wassiljiewa, Gambill, McAllister, Hind, Grunberg, Wijk, McAllister 4body, Tamura Kurata, Katti-Chaudhri and Nhaesi.

KEYWORDS: Viscosity; 1,4-butanediol; Ethanol; Excess Gibbs energy of activation; Viscosity relations.

THE KEY ROLE OF MENDELEEV'S FORCES IN INTERMOLECULAR INTERACTIONS

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Studies of organic liquids and various biological systems lead to the conclusion that the energy of intermolecular forces is a function of density ρ and is determined by three types of forces:

$$E_{p} = B\rho^{2} - a\rho^{4} + b\rho^{1/3}$$
⁽¹⁾

Here $B\rho^2$ is the energy of dispersive forces of attraction (m = 6), $-a\rho^4$ is the energy of repulsive forces (n = 12), and $b\rho^{1/3}$ is the energy of the binding forces of the particles determined by the long-range non-covalent Coulomb binding forces (k = 1) (proportional to the critical temperature of the substance. The dispersion force constant *B* as well as the bond forces *b* are determined by the critical parameters

$$\left(\frac{\partial p}{\partial T}\right)_{V}^{cr} = \frac{B\rho_{cr}^{3}}{T_{cr}} + \frac{R}{M}\rho_{cr}, \quad b = \frac{RT_{cr}}{2M\rho_{cr}^{1/3}}$$
(2)

Mendeleev was one of the first to draw attention to the existence of special bonding forces responsible for the association of particles of matter occurring in the critical region and later because of these bonding forces were called Mendeleev's forces.

Differentiating formula (1) by volume and taking into account the well-known ratio it was obtained the formula (3), which determines the pressure created by the molecules of the vapor phase. This formula, which determines the vapor pressure, is presented below.

$$p_{s} = \frac{1+\delta}{2} \frac{RT}{M} \rho - \delta \frac{1}{3} b \rho^{4/3} - 2B\rho^{3} + \delta 4A\rho^{5}.$$
 (3)

Formula (3) takes into account the action of each of the three types of forces by its derivatives from the energy caused by each of them. The association of vapor particles, caused by Mendeleev's forces, and the effects associated with it, are controlled by the dissociation coefficient δ , the value of which is determined by the equilibrium constant *K*, which in turn also depends on the value of the binding energy

$$K = C\rho T^{3/2} \exp(T_{cr}/T) = \frac{1-\delta^2}{4\delta^2} \Longrightarrow \delta = \frac{1}{\sqrt{4K+1}}.$$
(4)

As an example, the calculations of the saturated vapor pressure of different substances, carried out for the equilibrium curve, including the critical point. The value of the constant C included in the ratio for the equilibrium constant K was determined by normalizing the dissociation coefficient δ to 1/2 at the critical point.

The observed complete agreement of the calculated values of the saturated vapor pressure with the experimental data serves as a reliable proof of the objectivity of Mendeleev's forces and leads to the urgent need to take them into account when analyzing the results of predicting various thermophysical processes. They can be considered a reliable correcting factor that guarantees an adequate solution to numerous problems in the physics of the liquid state.

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EXPERIMENTAL INVESTIGATION AND 3D ANALYTICAL MODELLING OF LIQUIDUS SURFACES OF THE MnTe-SnTe-Sb(Bi)₂Te₃ SYSTEMS

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The complex long-period structure of magnetic and topologically non-trivial regions in manganese bismuth or antimony chalcogenides is considered a promising material platform for the realization of many interesting topological quantum phenomena, including quantum anomalous Hall effect, Majorana modes, and so on [1,2]. Ternary phases in the MnTe-Sb(Bi)₂Te₃ systems have a tetradymite-type layered structure and it consists of a repetition of septuple blocks where magnetic MnTe bilayers are inserted into the quintuple Sb₂Te₃ or Bi₂Te₃ layers periodically [3,4].

The knowledge on phase equilibria of corresponding systems provides essential information on the development of modern sample-preparation techniques and bulk single crystal growth via the determination of primary crystallization fields.

In this paper, we report an experimental investigation and 3D analytical modeling of liquidus surfaces of MnTe-SnTe-Sb(Bi)₂Te₃ systems. Constructed diagrams can be used when selecting the initial composition of the melt for growing single crystals of magnetic topological insulator phases.

The samples were prepared from pre-synthesized initial binary compounds – MnTe, SnTe, Sb₂Te₃, and Bi₂Te₃. Their synthesis was carried out by melting stoichiometric amounts of components in evacuated (\sim 10⁻² Pa) silica ampules at temperatures between 800 and 1100°C depending on the composition and subsequently quenched in ice water from the melt. Then all samples were annealed in the furnace at 700, 600, and 550 °C for 60 days to form equilibrium phases.

All samples were examined using differential thermal analysis (LINSEIS HDSC PT1600) and powder X-ray diffraction (Bruker D2 PHASER) techniques. Morphological characterizations of the samples were done by Tescan Vega 3 SBH scanning electron microscope. All analytical dependencies were obtained using the "analysis" option of the OriginLab software.

Based on obtained results, the liquidus surface projection of both systems was constructed. It was established that continuous series of solid solutions are formed in 2 sections, namely $MnB_2^{V}Te_4$ -SnB $_2^{V}Te_4$ and $MnB_4^{V}Te_7$ -SnB $_4^{V}Te_7$ (BV- Sb, Bi) in both systems. There is also a wide range of Mn \rightarrow Sn substitutional solid solutions based on $MnBi_6Te_{10}$, $MnBi_8Te_{13}$, $MnBi_{10}Te_{16}$, and $MnBi_{12}Te_{19}$ compounds. The primary crystallization areas of these phases, as well as types and coordinates of all non- and monovariant equilibria are determined. An analytical method was used for 3D modeling of crystallization surfaces of both systems and obtained dependences of the liquidus temperatures on the composition allowed us to visualize the crystallization surfaces.

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THERMODYNAMIC STUDY OF MANGANESE ANTIMONY TELLURIDES

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Recent studies show that intrinsic magnetic topological insulators provide great opportunities to study many novel topological phenomena including the quantum anomalous Hall effect which offers an essential chance for the development of low-power-consumption electronics. Naturally occurring magnetic layer contained tetradymite-type layered phases with $MnSb(Bi)_2Te_4$ ·($Sb(Bi)_2Te_3$)_n formula are intensively studied as experimentally realizable intrinsic magnetic topological insulators in the recent years [1,2].

The knowledge of phase equilibria and reliable thermodynamic data of corresponding systems are crucially important for designing and synthesizing novel complex phases. Here we studied thermodynamic properties of manganese antimony tellurides in the MnTe-Sb₂Te₃-Te composition region using EMF measurements with a liquid electrolyte.

Alloys of the MnTe-Sb₂Te₃-Te system were prepared using pre-synthesized initial binary compounds and elemental tellurium. A mixture of components was placed in the evacuated ($\sim 10^{-2}$ Pa) quartz ampules and synthesized at 1000 K for 5 h followed by quenching in icy water. The resulting ingots were furtherly annealed at 700 K for 45 days to form equilibrium phases. All alloys were examined using differential thermal analysis (LINSEIS HDSC PT1600 system) and powder X-ray diffraction (Bruker D2 PHASER diffractometer) techniques. EMF measurements were performed using a Keithley 2100 6 1/2 Digit Multimeter.

For EMF measurements, the concentration cell of

(2)

(3)

Mn+MnTe₂+4Sb₂Te₃=2MnSb₄Te₇ Mn+MnTe₂+2MnSb₄Te₇=4MnSb₂Te₄

Using these data and corresponding thermodynamic functions of MnTe and Sb₂Te₃, the standard thermodynamic functions of formation and standard entropies of the MnSb₂Te₄ and MnSb₄Te₇ compounds were calculated.



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CHARACTERIZATION OF ZWITTERIONIC PHOSPHORYLCHOLINE BASED BRUSH TYPE POLYMER CHAINS ON TITANIUM SURFACES BY SURFACE-INITIATED POLYMERIZATION AND ITS EFFECT ON MINERALIZATION

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Titanium and its alloys are widely used in the field of biomaterials, especially medical implants. The use of titanium and its allovs is common in the treatment of bone tissue and mass that disappear or lose function as the world's aging population, dental disorders, accidents and sports injuries increase. Mechanical properties such as Young's modulus, fatigue strength and corrosion resistance are the closest to the bone, and the implantation success of titanium is high, but the prospect of events that occur in the area as it contacts with tissue in the early period is also great. Although design and surgical techniques in implant science seem to be the most important steps in success, physiological events that make up the concept of biocompatibility take place at the interface between the tissue and the implant, so it is necessary to study the surface properties of the implant in detail. Wettability, protein adhesion, surface potential and topography are the main features of these properties. It is important that the interaction of titanium metal-based implants with tissues is increased, and that the surface properties of titanium are examined in the above-mentioned biocompatibility concept, and that these properties can be extracted at maximum levels of tissue-to implant compatibility for titanium metal implants. One of the various ways in which the surface properties of the titanium metal can be altered and controlled to enhance implant-tissue conformity is the growth of polymers over the surface, which is guite new in the literature. Surface-assisted atom transfer radical polymerization (SI-ATRP) is at the forefront of these techniques. In this study, it was aimed to increase the compatibility of the implant-tissue with phosphorylcholine-induced wettability, mineralization increase and cell proliferation effects by activating phosphorylcholine based brush type polymers from active functional groups formed on the titanium surface using SI-ATRP. The resultant modification has been demonstrated by various characterization techniques and cell culture studies that increase surface wettability and surface free energy, increase the amount of apatitic calcium phosphate, and positively affect osteoblast cell proliferation.

ANALYSIS AND MOLECULAR CHARACTERIZATION OF MATERIALS ORGANIC FOR APPLICATION IN SOLAR CELLS

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Organic solar cells represent a good alternative in obtaining energy. They are made from polymers, which form the matrix or the nanometric reinforcement responsible for the photovoltaic phenomenon; these materials are degradable or recyclable, which presents an improvement compared to conventional solar cells. Thus, the PCPDTBT/Fullerene/HDPE nanocomposite was studied using the hybrid method of molecular mechanics and quantum mechanics AMBER/PM3, where the calculations were, Gibbs free energy, bond lengths, electrostatic potential map (MESP), analysis Fourier transform infrared (FTIR) and the calculation of the molecular orbital (MO).

It was concluded that the negative Gibbs free energy indicated that there was an exothermic and stable process of the nanocomposite. On the other hand, the MESP showed that the nanocomposite can be susceptible to an electrophilic attack, the change in the coloration between nitrogen of PCPDTBT and the carbon of Fullerene indicated that there was a crosslinking between both molecules, which produced a new CN bond between them. The same situation was observed between the carbon atom (Fullerene) with a hydrogen (HDPE), which generated a new C-H bond. The FTIR analysis showed new signals of the new bonds, this confirmed the existence of the crosslinking and the stability of the nanocomposite molecule.

In the individual molecules, HDPE presented a band gap consistent with the bibliography, while PCPDTBT and Fullerene presented band gaps with higher values due to the considerations of the quantum mechanical method. Once the PCPDTBT/Fullerene nanocomposite was formed, the value of the band gap decreased due to a tendency to transfer electrons. When the polymeric matrix was inserted into the nanocomposite, the value of the band gap increased slightly due to the insulating property of HDPE.

However, once the molecule receives UV radiation, the value of the band gap decreased considerably until reaching values that are compared with conductive materials, indicating that there is mobility of electrons, and therefore, the polymeric matrix nanocomposite can generate electric current.

Keywords: solar cells, PCPDTBT, HDPE, Fullerene, nanocomposite, AMBER, PM3

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EFFECT OF EXPANDED GRAPHITE ON THE HEATING AND COOLING RATE OF THE PHASE CHANGE MATERIAL FOR THERMAL STORAGE

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Thermal energy storage (TES) plays an important role in heat power systems. Utilizing of phase change materials (PCMs) and selecting additives to enhance their thermal conductivity is a promising way to increase the efficiency and reliability of TES systems. Paraffin wax (PW) is an attractive material for TES applications, but it inherent a low thermal conductivity. Expanded graphite (EG) is one of the promising additives to PCMs for increasing their thermal conductivity.

The following materials as PCMs were used for studying: PW of industrial-grade with melting temperature 53.5 °C and PW containing 0.111 kg·kg⁻¹ of EG (GFG600, supplier the SGL Sigratherm, Germany, purity not less than 95 wt. %, D₅₀ determined by sieve analysis 200 μ m) - PW+EG. The method of PW+EG producing was based on EG heating (up to 700 °C) with vacuuming for 15 min, followed by mixing the pre-vacuumized molted PW (70-75 °C) and vacuuming of obtained composite PCM at 65 °C for 30 min. The density of PW and PW+EG (method of pycnometer of solid phase) were 900.5 and 930.2 kg·m⁻³ at 25 °C, respectively. The fraction of pores not filled with PW was 4.5 wt. %.

Since the measuring of the thermophysical properties of composite PCMs is time-consuming and expensive, the experimental investigations of heating (charging) and cooling (discharging) rates of capsule containing composite PW+EG are actual for estimation of its industrial expediency. In the presented study the rates of temperature change in pure PW and PW+EG were experimentally measured. The experimental cell was considered as a model of capsules of the TES system. The cell was produced from copper and has 12 mm in diameter and 110 mm in height. Two thermocouples were installed in the middle of the height of the cell (in the center and near the wall). Two liquid thermostats maintained different thermostating temperatures. Two modes of heating and cooling were studied: from 48 to 59 °C (the mode with a phase transition) and from 30 to 40 °C (the mode without phase transition). The obtained time dependence of the temperature in the measuring cell center is presented in Figure 1.



transition (left) and without a phase transition (right)

As we can see from Fig. 1, the PW+EG has a significantly higher heating rate vs pure PW. The obtained effects confirm the improvement in the effective thermal conductivity of the PW containing the EG. For the final interpretation of the results obtained the measurement of the thermal conductivity and caloric properties for PW and PW+EG is going to be performed.

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THERMOPHYSICAL AND CORROSION PROPERTIES OF AI-Ni-Co-R ALLOYS

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Aluminum-based metallic glasses (Al > 80 at.%) with 3d-transition metals (TM) and rare earth metals (REM) have unique physical properties, combining high strength and plasticity together with high corrosion resistance. Nowadays these alloys are used as protecting materials in industry. In this work we investigated thermophysical properties (density and electrical resistivity) and corrosion properties of Al-Ni-Co-R alloys in solid, liquid and amorphous states with the different Ni/Co ratio.

The alloys of Al₈₆Ni₄Co₄R₆ and Al₈₆Ni₆Co₂R₆ (R = Nd, Sm, Gd, Tb, Yb) compositions were prepared by remelting of pure initial components in arc-melting furnace in argon atmosphere. Amorphous ribbons were produced by planar flow casting method. Density of the alloys in crystalline and liquid states was measured by the absolute variant of gamma-absorption method on an automated experimental set-up in helium atmosphere. Electrical resistivity of the alloys in crystalline and liquid states was investigated by contactless method in rotating magnetic field on automated experimental set-up in helium atmosphere. Corrosion properties of amorphous samples were studied by gravimetric analysis in NaCI (5 wt.%) water solution at 293 K for 1500 hours. Electrochemistry was investigated by voltammetry method at potentiostat AutoLAB PGSTAT 30.

It was found that all the compositions have a wide two-phase zone (transition from solid to liquid state) and specific behavior of properties (density and electrical resistivity) at liquidus temperature. Hysteresis of density (i.e. incoincidence of heating and cooling curves) was found for all the alloys. The alloys with high cobalt content demonstrate the highest corrosion resistance. It was stated that Gd and Yb additions are preferable for increasing the corrosion resistance of the alloys.

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THE SYNTHESIS OF MIXED DIESTER OF NATURAL PETROLEUM ACIDS

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Esters of petroleum acids are widely used in various industries as solvents, plasticizers, lubricants and diesel fuel additives. This thesis is devoted to the synthesis of mixed propylene glycol diester based on natural petroleum acids (NPA) and capronic acid in the presence catalyst - ZnO. The synthesis of propylene glycol diester of NPA and capronic acid proceeds according to the following scheme:



where: R - radical of NPA, R'- C₅H₁₁-.

A series of experiments was carried out to find the optimal conditions for the synthesis of propylene glycol mixed diester. For this purpose, the following reaction parameters were varied: the molar ratio of acid:alcohol in the range of 2:1.3-1.6; the amount of catalyst 0.8-1.5% wt. to the taken acid; the reaction temperature range is 80-140°C. Further, the optimal mode was determined: the molar ratio of acid:alcohol - 2:1.3; the amount of catalyst - 1.3-1.5% wt. to the taken acid; reaction temperature - 110-120°C.

For the synthesis of propylene glycol diester of NPA and capronic acid, 112.2 g of NPA, 58 g of capronic acid, 49.4 g of propylene glycol, 2.55 g of ZnO and 155.5 g of toluene (taken in the amount of 70% of the total mixture of components) were taken. The end of the reaction was monitored by determining the acid number by periodical sampling. The value of acid number at the end of the reaction is determined by calculation based on the amount of taken catalyst. Upon completion of the synthesis, the reaction mixture was cooled to room temperature and the mixture was separated from the catalyst by filtration. After distilling off the solvent, the excess of the starting alcohol is distilled, and then the target product.

The resulting mixed diester has the following physicochemical parameters: $T_{\text{boil.}}$ - 190-240°C at P = 2.66 • 10⁻⁴ MPa, , n_D^{20} - 1.4572, ρ_4^{20} - 0.9825 g / cm³, acid number - 0.58 mg KOH/g, the number of saponification - 302 mg KOH/g, ester number – 301.42 mg KOH/g. The diester yield is 90.2%.

In laboratory conditions, compositions were prepared, consisting of 100 wf. PVC, 30-50 wf. mixed diester and 1 wf. stabilizer. Compositions prepared on the basis of dioctyl phatalate served as control samples. At temperatures of 65°C, 75°C, 85°C by keeping them for 6 hours in a thermostat until the optimal time for complete swelling of the PVC composition in a plasticizer, and it was found that the studied ester is well combined with PVC at 40 wf.

According to the degree of compatibility, the synthesized ester can be recommended for use as the new effective plasticizers for frost-resistant polymeric materials.

NEW INVESTIGATION OF PHASE EQUILIBRIA IN THE SnTe-Bi₂Te₃ SYSTEM

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An investigation of $A^{IV}Te-B^{V_2}Te_3$ ($A^{IV} = Ge$, Sn, Pb; $B^{V} = Sb$, Bi) systems has great importance in terms of searching high-performance thermoelectric materials, as well as a new quantum state of matter called "topological insulator" phases [1]. The latest studies confirm that ternary phases in these systems are three-dimensional topological insulators [2,3].

The knowledge of phase equilibria and reliable thermodynamic data of corresponding systems provide important guidelines for designing and synthesizing novel complex phases [1]. Although many authors have investigated the SnTe-Bi₂Te₃ system, its phase diagram is still controversial. All proposed versions of phase diagrams differ in several aspects, mainly the number of ternary compounds and their melting temperature. Therefore, an experimental re-investigation of the titled system seems worthy from the material science point of view.

Hence, in this paper, we re-studied the phase relationship of the SnTe-Bi₂Te₃ system in order to clarify discrepancies. Samples of the SnTe-Bi₂Te₃ system were prepared using pre-synthesized initial binary compounds: SnTe and Bi₂Te₃. Stoichiometric amounts of initial components were placed in the evacuated (~10⁻² Pa) quartz ampules and synthesized by fusion at temperatures of 650-900°C for 5 h depending on the composition. Then all liquid samples were quenched in ice water. The resulting ingots were furtherly annealed at 550°C for 45 days to form equilibrium phases.

All homogenized samples were characterized using differential thermal analysis (SETARAM Instrumentation system), powder X-ray diffraction (Empyrean diffractometer), and scanning electron microscopy (Hitachi SU8020) techniques. According to PXRD and SEM analysis, the existence of three tetradymite-type layered ternary compounds, SnBi₂Te₄, SnBi₄Te₇, and SnBi₆Te₁₀ was confirmed. All listed ternary compounds melt with peritectic reaction at 597, 590, and 586 °C, respectively. In contrast to the published complied diagram in [4], we observed approximately 12 mol% homogeneity region based on SnTe and 10 mol% based on Bi_2Te_3 at low temperatures. Previously reported $Sn_2Bi_6Te_{11}$ and $SnBi_8Te_{13}$ compounds were not observed in our studies.

807 800 Ē, SnBi₄Te₇ SnBi₆Te₄ SnBi, 700 L+ε L+β L+α L+δ p 597 600 p. 587 586 575 e α 550 δ β 3+2 500 $\gamma + \delta$ β+ε $\alpha + \gamma$ Bi₂Te₃ SnTe 20 40 60 80 mol% Bi,Te,

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SALTING-OUT OF BUTYRIC ACID FROM AQUEOUS SOLUTIONS WITH SODIUM DIHYDROGEN PHOSPHATE IN THE RANGE OF 10–40 °C

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Butyric acid finds important applications on the markets of solvents and polymers, as well as in the food, cosmetic and pharmaceutical industries. Currently, most of this acid is produced from petrochemical products using a catalytic oxidation process. An alternative ("green") method for producing butyric acid is obtaining from solution by fermentation. This kind of the acid is called biobutyric acid and is widely used in the cosmetic, pharmaceutical and food industries, since it contains no organic synthesis by-products harmful to the body. The production of biobutyric acid is complicated by its low content in fermentation solutions (below 80 g/L), which requires searching for effective methods for its concentrating. To optimize the salting-out butyric acid under the action of salts at different temperatures. Analysis of such data allows one to give recommendations on the conditions for carrying out concentrating and isolation to achieve the maximum efficiency of these processes. The aim of this work was to reveal the phase behavior of mixtures of water and butyric acid under the action phosphate in a range of 10.0÷40.0°C.

Phase equilibria in mixtures of the components of the ternary system sodium dihydrogen phosphate + water + butyric acid, whose compositions varied along eight sections of the concentration triangle, were studied by the visual polythermal method in a temperature range from 10 to 40° C. Sections I–V were characterized by a variable salt content and a constant mass ratio of butyric acid and water: 7.00:93.00 (I), 30.00:70.00 (II), 50.00:50.00 (III), 68.00:32.00 (IV), and 81.50:18.50 (V). The polytherms of phase states along sections I–V were similar. Each of them consists of two curves separating the fields of homogeneous solutions from the separation field, and the separation field from the monotectic field (the solid phase being NaH₂PO₄·2H₂O).

The component mixtures in sections VI and VII were characterized by a variable content of butyric acid and a constant mass ratio of sodium dihydrogen phosphate and water: 32.00: 68.00 (VI) and 60.00:40.00 (VII). The component mixtures along section VIII were characterized by a constant salt content and a variable content of a water-butyric acid mixture: 9.00:91.00 (VIII). Isothermal phase diagrams of the ternary system at 10.0, 20.0, 25.0, 30.0, and 40.0°C were plotted on the basis of polythermal data. In the range of 10.0–40.0°C, the phase diagram of the ternary system is characterized by the presence of a monotectic triangle with an adjacent separation field and adjacent fields of saturated solutions. A set of phase states occurs within this temperature range, which is characteristic of isotherms of ternary systems with salting-out of mixtures of a binary homogeneous system. As temperature rises, the phase diagrams differ qualitatively only, namely: the area of the monotectic triangle decreases, while the stratification field area increases.

The obtained isotherms made it possible to graphically estimate the composition of the equilibrium phases of monotectic state and calculate the distribution coefficient K_d of butyric acid at 10.0, 20.0, 25.0, 30.0, and 40.0°C. The distribution coefficient increases with temperature (K_d = 78 and 235 at 10.0°C and 40.0°C, respectively), which indicates an enhanced effect of salting-out butyric acid from aqueous solutions with sodium dihydrogen phosphate is an effective salting-out agent and allows butyric acid to be concentrated from dilute aqueous solutions.

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PRECISE PVTX AND VLE PROPERTY MEASUREMENT FOR LOW-GWP REFRIGERANT MIXTURES

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Several low-GWP type refrigerants and their mixtures are expected as next generation refrigerants alternatives to the existing refrigerants that have heavy greenhouse effect. Especially a variety of three-component and multicomponent refrigerant mixtures mixing with binary pairs with R1123, R1234yf, and R32 are expected as nextgeneration refrigerant candidates to provide decreasing of the flammability and/or toxicity, increasing of the compatibility with lubricating oils. For the common prediction of the ther-modynamic properties for more than ternary mixtures, only parameters for pure and binary mixtures (without any additional parameters for more than ternary mixtures) are adopted. We therefore try to evi-dent the enough reliability of these prediction based on the comparisons between the widely available models and the precise measurements of the thermodynamic properties by the present study.

We used two kinds of models in the present comparisons. One is the Helmholtz-type models, which are adopted in the most recent REFPROP ver.10.0 ^[1]. We predicted the vapor-liquid equilibrium (VLE) property data of the ternary mixtures by REFPROP ver.10.0. The other is the present Peng-Robinson equation of state ^[2] modified by Mathias and Copeman ^[3]. The required parameters of the pure and binary fluids for the ternary calculations have been determined by the group of the present authors. On the other hand, the experimental data are measured by means of the two kinds of the apparatuses, the metal bellows-type isothermal *PVTx* property measurement apparatus and the re-circulating type VLE property measurement apparatus, for the R1123/R1234yf/R32 ternary mixtures. The present measurements ranges are 5 to 55 °C for temperatures and up to 6 MPa for pressures. The expanded uncertainties (*k*=2) in temperature, pressure, density, and component measurements of the apparatus for the *PVTx* property measurements are estimated to be less than 3 mK, 1.4 kPa (*P*<6.9 MPa), 0.1%, and 4.1 \times 10⁻⁴, respectively. The systematic comparisons between the predicted values and the present measurements for the ternary mixtures will be reported.

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THERMAL EFFECTS ON DECAYING CADAVERS AND POSTMORTEM INTERVAL

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Thermal changes effect human corpses as much as they effect living human metabolism. While it is a well-known fact that frozen corpses can remain intact for a long time without any damage, it is also known that temperatures above freezing have different effects on the decomposition and decaying process of the corpse. Knowing the effects of temperature on the corpse plays a major role in determining the postmortem interval, which defines the period between death and the postmortem examination.

The response to thermal effects differs compared to homogeneous objects, since heating and cooling of the multilayered human corpse differs due to having each layer of the body varying thermal properties. This difference becomes a bit more complicated to predict, since metabolism continues for a while after death and releases a limited amount of thermal energy. For this reason, different formulations have been developed, accompanied by first linear and parabolic curves, then nomograms, and finally different scoring systems for postmortem interval determination by thermal effects. In this paper, the evolution of postmortem interval determination is discussed based on the relationship between the corpse and the ambient temperature from past to present.

KEYWORDS: Postmortem interval, decaying, body cooling

INTENSIFICATION OF THE ADSORPTION OF GAS MIXTURES WITH VARIABLE PRESSURES

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In modern chemical technology, adsorption devices are widely used for the interaction of substances in various states of aggregation. The desire to intensify the operation of industrial adsorbers leads to an increase in the speed of phase movement, an increase in local and average temperature gradients and pressure drop in the active zones of adsorption devices.

This work is devoted to the study of the process of adsorption of H₂S/CO₂/N₂ gas mixtures with variable pressure. Particular attention is paid to studies of a fixed bed of natural zeolite in a certain limit of pressure drop and the dependence of the flow rate of the incoming gas, which ensures the full use of the adsorption capacity of the zeo-lite. Work on the intensification of industrial adsorbers, despite numerous studies, has been insufficiently studied and is still relevant. A review and analysis of the technology of purification of gas mixtures from unwanted components is carried out. According to the results of the experiment, it was found that the adsorption of gas mixtures, at a linear flow rate of 0.15 m/sec and maintaining a pressure drop in the adsorption layer of 21.7 kPa, the degree of unused adsorption capacity of clinoptilolite approaches 7.8%. As a result, at the outlet of the adsorber, respectively, residual concentrations of H₂S-0.028%, CO₂-0.01%, N₂-0.046% were obtained. The coefficients of the equations are found by calculations based on the "Matlab" system in the "Optimization Toolbox" environment. Thus, the system of equations which was shown in article, describes the adsorption of the components of gas mixtures in a fixed bed of adsorbent, constitutes a complete mathematical model of the dynamics of the process under consideration in non-equilibrium conditions. The proposed formulas can be used in the study and calculations of industrial adsorbers in conditions with variable pressure.

THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES FOR GREEN COMPOUNDS AT HIGH PRESSURES

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The harmful impact of the fossil fuels consumption on the environment and their limited reserves have prompted a reaction from both researchers and government officials. New environmental protection measures have been adopted and the research for renewable energy sources is strongly supported. The goal is to find the renewable, non-toxic, biodegradable, environment-friendly substitutes for fossil fuels and optimize their use. Within our research various green solvents and biofuels, such as biodiesels, terpenes, ionic liquids, and deep eutectic solvents have been studied. Biodiesels are widely known substitutes for fossil fuels; they can be applied in diesel engines, pure or mixed with a petro-diesel in various proportions, without corrections in engine design [1]. Terpenes found a promising role as an alternative fuel for aviation transport where fuel of high energy density is required due to small volume-limited fuel tanks [2]. Ionic liquids have shown a great potential in CO₂ absorption from air or exhaust gas. These salts are very attractive for industrial purposes, because of their specific properties, changed based on selected combination of anion and cation [3]. Further, for more efficient energy production and consumption, investigation on improving the properties of the heat transfer fluid was performed, adding nanoparticles to ethylene glycol (EG) [4].

The data on thermophysical properties of various chemical compounds and their mixtures under different conditions of pressure and temperature are essential for various processes. For example, the fuel injection and combustion in diesel engines are performed at high pressures and temperatures and are greatly influenced by the fuel's density and viscosity [1].

Densities of sunflower oil biodiesels and their mixtures with diesel fuel, a group of terpenes and ionic liquids, and EG with caffeine were measured at temperatures in the range (298.15–413.15) K and at pressures up to 60 MPa [1-4]. The experimental data were successfully correlated using the modified Tammann–Tait equation. That enabled the calculation of the derived properties, such as the isothermal compressibility, the isobaric thermal expansivity, the internal pressure and the difference between the specific heat capacity at constant pressure and at constant volume.

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TYPIFICATION OF NEAR-CRITICAL FORMATION FLUIDS BY INTENSITY OF CRITICAL OPALESCENCE ON THE DEW-BUBBLE BOUNDARY CURVE

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According to API, there are four types of near-critical formation fluids that are in the reservoir before its development in a single-phase state: volatile and very volatile oil, rich and very rich condensate gas. However, a clear criterion for the typification of these fluids, tied to their phase diagrams in the vicinity of critical points, still does not exist due to the lack of a practical criterion for classifying fluids as near-critical and critical types.

On the basis of optical measurements, a new method is proposed for identifying the near-critical and critical state of a fluid and, on its basis, for typification of near-critical formation fluids by the intensity of critical opalescence on the boundary dew-bubble curve. The idea of the method is to measure the intensity of Rayleigh light scattering in a single-phase region near the liquid-gas critical point and to determine the boundaries of the near-critical and critical regions in the form of contours, where the intensity of light scattering is an order of magnitude and two orders of magnitude higher than the intensity value far from the critical point. The latter is taken to be the value of the intensity of light scattering at a critical value of temperature and pressure, say, 10% higher than its critical value. The temperatures of the points of exit of these contours on the boundary curve are taken as the temperature boundaries of the critical and near-critical regions, which, together with the critical temperature value, determine the temperature intervals corresponding to different types of near-critical formation fluid. The described procedure is illustrated by the example of a model binary mixture methane-pentane and a recombined formation hydrocarbon fluid, consisting of samples taken from a real oil and gas condensate field.

The aim of the work is to draw attention to the problem of typification of near-critical formation fluids according to the phase diagram and stimulate discussion about possible ways of its solution.

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UNIVERSATITY IN THE EXPANSION ISOLINES BEHAVIOR AND THE THERMODYNAMIC CURVATURE

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The understanding of behaviour of volumetric properties of compressed liquids is in a field of great interest because of its crucial importance in representing liquid's derivative properties in both experimental- and theorybased Equations of State (EoS). At the same time, the lack of direct experimental PVT measurements at high pressures makes challenging the production of highly accurate EoS', valid in a wide range of pressures. In such cases, the solution may be in the introduction of new criteria of validity, based on the search of general rules for high order derivatives of volumetric properties.

In the present study, we consider the temperature dependence of the thermal expansion coefficient α_P of liquids in the region of elevated pressures below the critical temperature, which can change its sign depending on the external pressure, from the point of view of the Riemannian thermodynamic curvature R and the molecular packing ratio ρ^* . In particular, the behaviour of the curve $(\partial \alpha_P / \partial T)_P = 0$, separating the regions of increasing and decreasing α_P , was studied for 15 substances, different as by the shape of molecules as by the chemical composition extending the consideration proposed in the work [1].

It was shown that the exploration of the interplay of the thermodynamic curvature and the curve $(\partial \alpha_P / \partial T)_P = 0$ is the clearest on the (ρ^*, T) -plane, where the *R*-isolines form a set of almost straight lines, and the curves $(\partial \alpha_P / \partial T)_P = 0$ are concentrated within also almost linear narrow stripes. Thus, it was found that the curves $(\partial \alpha_P / \partial T)_P = 0$ provide a criterion, which allows for estimating the correctness of thermodynamic data representation at high pressures. Moreover, the shape of molecules can provide additional information on the location of $(\partial \alpha_P / \partial T)_P = 0$ curve for non-polar substances, which either belongs to the stripe of the spherical-symmetric molecules or the stripe chained ones, which is also valid for branched isomers.

The discussion of obtained results was carried out by employing the interpretation of the thermodynamic curvature as both the measure of average intermolecular interactions and the volume where the intermolecular forces cause a considerable contribution in fluctuations of the density of liquid [2]. We consider the effects of tending to the random close packing at freezing and for small molecules and relatively long-traced coincidence of isolines of $(\partial \alpha_P / \partial T)_P = 0$ and R under this condition for the long-chained molecules. In addition, possible effects of polarity are shortly discussed.

The obtained general boundary values of R were explained geometrically from the point of view of a closepacked binary mixture of spheres associated with effective molecular segments and voids that also argues the connection of the thermodynamic curvature to the reduced free volume in the non-critical region.

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NISIN LOADED DNA ORIGAMI: ANTIMICROBIAL AND CYTOTOXIC ACTIVITY STUDIES

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DNA Origami is a common technique to form 2D and 3D nanostructures, in which a long single-stranded oligo is being folded by short 'staple' strands. Lantibiotics are rybozomilly synthesized peptides having potential as medically significant antimicrobial and anticancer agents. Nisin is a well known antibacterial member of lantibiotic family used as food preservative.

In this study 60 Helix Bundle DNA nanostructures are built in DNA Origami method prepared by described earlier [1], thermal annealing of folding solution with a long 'scaffold' DNA mixed with 141 distinct staple DNAs. The excess amount of staples were removed by PEG-based purification. Folding and purification of DNA origami is characterized by Transmission Electron Microscopy. Nisin loaded with DNA in 150/1 molar ratio. Antimicrobial tests performed with BSA addition to avoid binding nisin to microtiter plate and washed with water prior to use for TAE Buffer removal.

Antimicrobial activity of Nisin loaded DNA nanostructures tested against Methyciline Resistant Staphylococcus aureus (MRSA) and Vancomycine Resistant Enterococcus (VRE) and showed as less as 13% and 22% viability with bare nisin and 23% and 8% viability with nisin loaded DNA Origami respectively. No effect observed with bare DNA as expected. Moreover in MTT tests nisin and nisin loaded killed up to 50% of MCF-7 human breast cancer cells and only killed 20% of L929 Mouse fibroblast cells.

The study on the antimicrobial and cytotoxic activity of nisin loaded DNA origamis showed the great potential of lantibiotics as an promising alternative to the antibiotics to the resistant bacterias and its potential as an anticancer agent. Also DNA Origamis showed straightforward solution as an alternative to nanoparticle, polymer and virus based carriers. This study created from part of Aykut Bilir's ongoing PhD thesis in Division of Nanotechnology and Nanomedicine, Hacettepe University.

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DENSITY, SPEED OF SOUND, REFRACTIVE INDEX AND RELATED DERIVED/EXCESS PROPERTIES OF BINARY MIXTURES (FURFURAL + DIMETHYL SULFOXIDE), (FURFURAL + ACETONITRILE) AND (FURFURAL + SULFOLANE) AT DIFFERENT TEMPERATURES

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Furfural is one of the furan derivatives produced from the hemicellulosic fraction of lignocellulosics, which is considered a promising commodity bio-based chemical because of the possibility of its use in the production of several products as paints, fertilizers, fuel additives and many others products. The present work is part of research work on physicochemical, thermodynamic, and thermophysical properties of mixtures containing components derived from biomass.

In this paper, we report the experimental densities, speeds of sound, and refractive indices for three binary mixtures: (Furfural + Dimethyl Sulfoxide (DMSO)), (Furfural + Acetonitrile or (Furfural + Sulfolane) measured over the entire composition range and in the temperature range (293.15 to 313.15) K at 10 K intervals and at pressure p = 0.1 MPa. From the experimental data, excess molar volume, isentropic compressibility, excess isentropic compressibility, refractive index deviation, excess refractive index, molar refraction, molar refraction deviation, intermolecular free length, specific acoustic impedance, relative association, relaxation strength, and Rao's molar sound function have been calculated over the entire composition range and at each temperature.

Excess molar volume, excess isentropic compressibility, excess speed of sound, excess refractive index, and molar refraction deviation data have been correlated using the Redlich-Kister equation. The thermodynamic properties have been discussed in terms of the nature of molecular interactions between the components of the mixture.



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