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LIST OF POSTER PRESENTATIONS

(only corresponding author is listed)

Org. No.	Surname	Name	Title
1	Becker	Tim	Molecular simulations to estimate high temperature solubility data of NH ₃ /IL working pairs for double-effect absorption heat pump cycles
2	Bertrand	Murielle	Modelling of krypton-xenon separation by dynamic fixed-bed adsorption on zeolite
3	Bertrand	Murielle	Thermodynamic study of uranium oxalate precipitation: solubility and supersaturation ratio determination
4	Camacho Vergara	Edgar Luis	Adsorption and interfacial tension of inhomogeneous fluids with classical density functional theory approaches
5	Crespo	Emanuel	Glymes as an alternative solvent for gas processing.
6	Cripwell	Jamie	Exploring the applications of a discretised approach to parameter regression in SAFT-VR Mie
7	De Angelis	Maria Grazia	Modelling facilitated transport in Polyvinyl amine (PVAm) membranes for CO ₂ capture: insights from Molecular Dynamics and PC-SAFT EoS.
8	De Angelis	Maria Grazia	Atomistic simulation of local segmental dynamics and gas diffusion in CO ₂ -polystyrene systems
9	Di Nicola	Giovanni	Analysis of VLE of HFOs, HCFOs Blends with Cubic Equations of State
10	Domańska	Urszula	Separation of heptane/ethanol with ionic liquids. Ternary liquid-liquid phase equilibrium data
11	Domańska	Urszula	Ternary LLE measurements for the separation of ethylbenzene/styrene with ionic liquids

Org. No.	Surname	Name	Title
12	Emelyanova	Ksenia	Molecular thermodynamic modeling of spontaneous bilayer perforation in aqueous salt solutions of mixed surfactants
13	Enders	Sabine	Gas Solubility in Semicrystalline Polymers – Cavitation Stress Theory coupled with Sanchez-Lacombe EOS
14	Goutaudier	Christelle	Octanol-water partition coefficient of phthalates: Comparison between experimental and calculated data
15	Haarmann	Niklas	Heterosegmental Modeling of Thermodynamic Properties of Long-Chain Molecules using PC-SAFT
16	Haghbakhsh	Reza	Natural gas sweetening using a green solvent in the pressure swing process
17	Haghbakhsh	Reza	Experimental investigation of solubility of some aliphatic and aromatic hydrocarbons in a deep eutectic solvent
18	Iakovleva	Ekaterina Alekseyevna	Effect of sugar additive on partition behavior of bioorganic compounds in aqueous biphasic systems containing nonionic surfactant Triton X-114
19	Jamali Rafsanjani	Asma	Comparing the results of two different approaches to represent fluids properties in the wide range of PVT values
20	Knierbein	Michael	High-Pressure Influence on an Organocatalytic Reaction
21	Korchak	Petr	Partitioning behavior of L-tryptophan in aqueous-salt biphasic systems formed by water-miscible alkylimidazolium ionic liquids with different anions
22	Koulocheris	Vassilis	Predicting the solubility of mercury in hydrocarbons, compressed gases, water and methanol with the UMR-PRU model

Effect of sugar additive on partition behavior of bioorganic compounds in aqueous biphasic systems containing nonionic surfactant Triton X-114

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Nonionic ethoxylated surfactants are surface-active compounds that tend to become insoluble in water when heated above the certain temperature called cloud point temperature (CPT). These particular characteristics of nonionic surfactants, their biocompatibility and low toxicity gave rise to many applications, specifically to extraction processes (cloud point extraction, CPE). One of the widely used extracting agents is (1,1,3,3-tetramethylbutyl)phenyl-polyethylene glycol (Triton X-114) due to its low CPT.

It is well known that different additives (salt, sugar etc.) or pH value may affect CPTs and the thermophysical characteristics (density, viscosity) of nonionic surfactant systems [1]. This has a particular meaning for enzymatic reactions as highly sensitive to temperature or pH changes.

In the present work, the aqueous biphasic systems containing Triton X-114, L-arabinose and salt buffer ($\text{KH}_2\text{PO}_4/\text{K}_2\text{HPO}_4$) are considered as reaction medium for enzymatic hydrolysis of penicillin G (Pen G) to phenylacetic acid (PAA) and 6-aminopenicillanic acid (APA). The chemical equilibrium of this bioreaction is shifted to the products in case of effective extraction of PAA into surfactant-rich phase [2]. CPTs and the partition coefficients P_{mw} of solutes (Pen G, PAA, APA) are under investigation. The data on P_{mw} were obtained at 310,2 K and pH=4,3 providing the highest velocity of the bioreaction.

The results show that CPTs decrease at increasing concentration of L-arabinose. PAA also causes significant reduction of CPT while APA has a negligible effect on it. The data on partition coefficients show that L-arabinose as additive improve extraction of PAA to the surfactant-rich phase.

HPLC analysis was carried out on the equipment of the Research park of St. Petersburg State University, Center for Chemical Analysis and Materials Research. This study was financially supported by RFBR according to the research project # 16-53-12029a.

References

1. E. Ritter, R. Racheva, S. Jakobtorweihen, I. Smirnova // *Chem. Eng. Res. Des.* **121**, 149–162 (2017)
2. Z. Wang, L. Wang, J-H. Xu, D. Bao, H. Qi // *Enzyme Microb. Technol.* **41**, 121–126 (2007)