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BOOK OF ABSTRACTS

SYNCHROTRON RADIATION AND SMART NANOMATERIALS

SMART MICROFLUIDICS 2024



2-3 OCTOBER

SOCHI

SOUTHERN FEDERAL UNIVERSITY

**SMART MICROFLUIDICS
2024**

International conference

Book of abstracts

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This book of abstracts contains the results of the reports presented at the 1st international scientific conference "Smart Microfluidics" 2024. The fields covered catalytic approaches for the synthesis of functional materials, the development of microfluidic systems using the additive DLP approach for 3D printing, as well as practical approaches to the application of microfluidic technologies for the synthesis of novel functional materials in various fields of industry, chemistry and medicine.

Creation of effective electrocatalysts for hydrogen energy: composition, microstructure, application of microfluidic technologies in synthesis

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Electrocatalysts based on platinum nanoparticles are widely used in hydrogen energy, for example, to produce hydrogen by electrolysis (on cathode of proton-exchange membrane electrolyzers) and convert hydrogen into electricity (on anode and cathode proton-exchange membrane fuel cells). The development of scalable methods for producing platinum-containing nanostructured electrocatalysts and the selection of highly effective materials is an urgent task in the field of alternative energy. Liquid-phase or wet-synthesis methods are widely used to produce electrocatalysts. The conditions of wet-synthesis affect the microstructure and, accordingly, the electrochemical characteristics of the resulting materials. The transition to microfluidic and flow technologies for the production of electrocatalysts is due to the need to minimize costs associated with the volume of reagents used, reduce the use of energy resources and labor costs, and reduce the amount of waste in the production of the material. Also, in the future, the flow technology for producing electrocatalysts makes it possible to easily change production volumes depending on market needs, as well as scale it up if necessary. The research work is aimed at studying the possibility of using the flow synthesis method to obtain nanostructured electrocatalysts for low-temperature fuel cells. The aim of the study is to optimize the technological conditions for the synthesis of colloidal platinum nanoparticles and Pt/C electrocatalysts based on them.

The research is being conducted jointly with the laboratory "New Materials for Electrochemical Power Engineering" of SFedU, the Center for Science-Intensive Instrumentation of SFedU and the commercial partner PROMETHEUS R&D LLC.

This research was financially supported by the Ministry of Science and Higher Education of the Russian Federation (State assignment in the field of scientific activity N^oFENW-2023-0016).

Catalytic approaches for synthesis of functional organosilicon materials using microfluidic systems

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Catalysis plays a key role in modern organic chemistry. Catalytic approaches allow to obtain both bio-based and previously unknown complex structures.

Unfortunately, catalytic methods for the synthesis of functionalized organoelement compounds, in particular organosilicon, are less developed, compared to organic ones. At the same time, organosilicon compounds are among the most important, because of their wide applicability.

In this presentation main achievements of our research group will be discussed:

- Catalytic systems for the liquid phase aerobic Si-H- and C-H-functionalization, which allow obtaining a range of silanols [1,2], p-carboxyphenylsilanes [3,4] etc. Dumbbell-shaped and graft siloxane polymers were obtained based on silanols [5]. A variety of HOFs and MOFs were obtained based on p-carboxyphenylsilanes.

- Catalytic systems for ultra-fast silica-aerogel production. It allows to obtain high quality aerogels within 6-24 hours, compared to previous techniques, which require at least several days [6].

- [Pt]- and [Mn]-based catalytic systems for hydrosilylation. [Pt]-systems were shown to be recyclable up to 60 times [7-9]. [Mn]-system presents an alternative to expensive [Pt]-catalysts [10].

- Upscaling these processes, mainly using microfluidic systems [10,11].

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Features of fluid flow simulation in microchannels with internal structures

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The study of viscous fluid flows in microchannels with complex structure is important in the design of specific elements of microfluidic heat exchangers. Micro heat exchangers are devices in which fluid flows through various structures to remove heat from the device. The cooling efficiency depends on the characteristics of the fluid, the production material, and the parameters of the channel geometry through which the fluid flows. This work is focused on the study of the microchannel geometry influence on its flow capacity, which affects the efficiency of the heat transfer process.

Single-phase and two-phase flows in a microchannel with a complex internal structure at low Reynolds numbers are considered. The fluid flow is described by the Stokes equation without inertial forces and the continuity equation. The problem is solved using the three-dimensional accelerated boundary element method (BEM) [1].

In the research, the flow patterns of fluid with and without dispersed particles distributed in it are obtained. The influence of spatial arrangement, shape and total surface area of the internal structures of microchannels on their flow capacity is studied. The most optimal configurations of microchannels are shown for further design of functional elements of microfluidic heat exchangers to ensure their efficiency with the use of fewer resources.

The investigation was financially supported by Russian Science Foundation (№ 24-19-00697 <https://rscf.ru/project/24-19-00697/>).

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Microfluidic synthesis of vinyl iodide and online diagnostics of reaction products

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Microfluidic synthesis based on manipulates a small amount of fluids using channels with sizes ten to hundreds micrometres have formed new approaches to chemical engineering.[1]

In this work, we performed optimization gas and liquid flows for synthesis of vinyl iodide taking place on the surface of commercial Pt nanocatalyst (K_2PtCl_6 , Sigma Aldrich) in presence of NaI and the addition of acetylene using the microfluidic system. First, we carried out several classic experiments in a flask, then we moved on to microfluidic synthesis analyzing reaction products by mass-spectroscopy to compare the effectiveness of this approach.

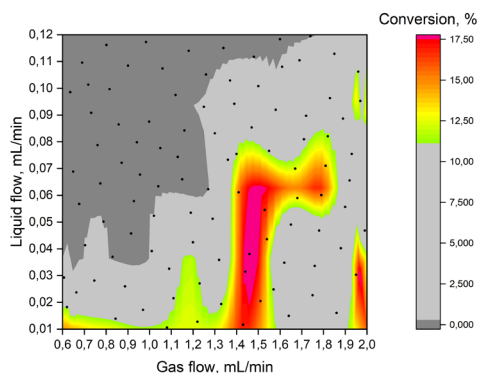


Fig. 1. Map of reaction conversion distribution.

The ratios shown in grey are worse than the classical method

As a result, we obtained improved solution for more effective way to synthesize vinyl iodide.

Acknowledgement

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Experimental studying of the fluid flow in the microfluidic chips with different pin packing parameters

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Latest developments in the field of microelectronics, genetic engineering and micromechanical device manufacture have led to creating a new branch of science called microfluidics, which is aimed at investigating the liquid system's behavior on a microscopic scale (from 1 μm to 100 μm). Microfluidic platforms are widely used in biochemistry, medicine, oil and gas industry. Nowadays, one of the most relevant problems is micro heat sink constructing as well.

The present work is devoted to studying the influence of the spatial arrangement of the inner structure elements in planar rectangular channels on hydrodynamic characteristics and channel capacity of the microfluidic device element. The microchannel structure plays a significant role as it must provide greatest possible heat transfer surface and acceptable hydrodynamic losses at the same time. The laboratory experiments with different PDMS chip configurations with fixed value of the total void were provided using the optical microscopy and tracer imaging techniques. The micromodel structure parameter influence on the flow distribution between the domains with different channel hydraulic diameters was investigated.

The investigation was financially supported by Russian Science Foundation (N^o 24-19-00697 <https://rscf.ru/project/24-19-00697/>).

Microfluidic synthesis of iron oxide nanoparticles

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Iron oxide nanoparticles could be used as anode materials [1] in lithium-ion (L-i) batteries due to its chemical properties and high availability. Fe_2O_3 can efficiently accept and release L-i charges, enabling it to store energy. Additionally, iron oxide has a theoretical capacity (up to 926 mAh/g), which significantly exceeds that of traditional graphite anodes (~372 mAh/g) [2]. This makes the use of iron oxide in batteries both relevant and promising.

In this work, a synthesis method was developed and optimized using microfluidic systems (MFS). The developed chip allows the use of membranes for syringes as a flow separator into small droplets, which serve as reaction zones, inside which magnetic nanoparticles (MNPs) of the same size are formed. The reaction of MNPs formation occurs instantly. Using MFS allows you to divide streams into small reaction zones and avoid clogging channels. During the synthesis, reactant concentrations were optimized to achieve the best reaction yield and particle morphology. The MNPs were characterized using a set of laboratory and synchrotron methods. X-ray powder diffraction suggests $\text{Fd-}\bar{3}m$ cubic structure, while X-ray absorption near-edge structure spectroscopy shows Fe^{3+} leading to $\gamma\text{-Fe}_2\text{O}_3$ phase. Transmission electron microscopy reveals spherical morphology with an average size of 60.8 nm. Fourier transform infrared spectroscopy tracks Fe-O vibrations. The magnetometry of the vibrating sample shows a high magnetization, 602.5 emu/g.

The authors acknowledge the Ministry of Science and Higher Education of the Russian Federation for financial support (Agreement № 075-15-2021-1363).

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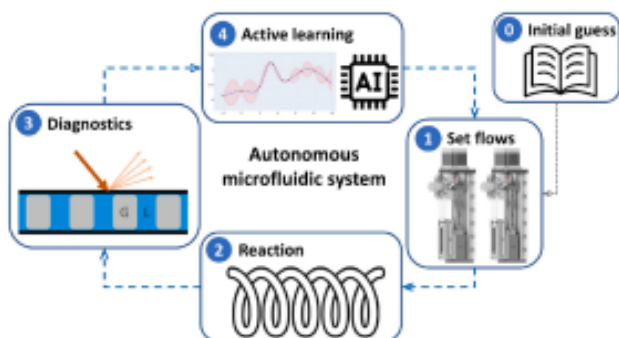
Microfluidic technology: physical processes, spectral diagnostics, and review of practical applications in chemistry

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Microfluidic systems offer unique capabilities for high-throughput screening. Reduced reagent consumption and the ability to quickly change the composition of incoming streams and the operating mode make microreactor systems convenient for screening the influence of many parameters on product yield and process selectivity. Feedback in the autonomous system is provided by spectral data measured from the capillary in situ. The development of new spectral monitoring cells and their integration with microfluidic systems allows online monitoring of both the composition of the reaction mixture via IR-Fourier and Raman spectroscopy methods and the state of metal centres by using X-ray absorption spectroscopy. In this work we discuss in details microfluidic realization and integration of spectral monitoring to industrially important homogeneous catalytic reactions.



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Synthesis of Biologically Active Compounds and Online UV-Vis Diagnostics in Microfluidic Chips

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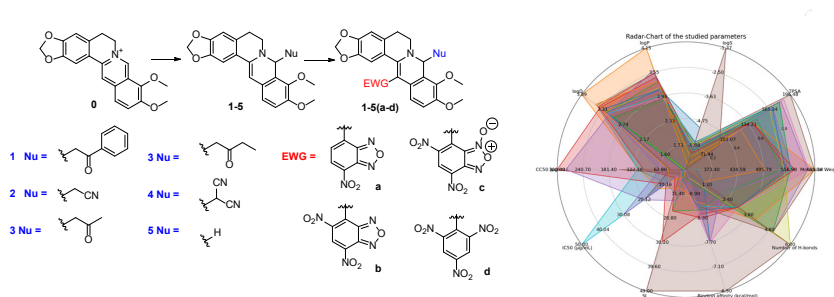
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Microfluidic technologies, being among the most advanced in scientific research, play an increasingly significant role in various fields of science, including fundamental and applied areas. They enable researchers to effectively address a range of complex problems that they frequently encounter. Among these problems are ensuring the representativeness of chemical syntheses, preventing errors in experimental methodology, scaling processes, reducing costs and reagent consumption. Moreover, microfluidics possesses several unique advantages that cannot be realized in traditional laboratory conditions.

We successfully realized the synthesis of new compounds that exhibit antiviral activity, specifically against the *Influenza A virus*, in a flow regime. In addition, we conducted studies on the antiviral activity of these compounds both *in vitro* and *in silico*.



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Microfluidic assisted Bio mineralization of Calcium Phosphate: Enhancing Particle Design

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Calcium phosphate (CaP) polymorphs are non-toxic and compatible with biological systems, which makes them appealing for various uses, such as in the regeneration of hard tissues, drug delivery, and vaccine formulation. Understanding the processes behind calcium phosphate nucleation and growth is essential for addressing diseases linked to abnormal mineralization and for creating biomimetic materials with desirable characteristics. The existing in situ or batch biomineralization methods for CaP typically follow a crystal formation pathway that involves the aggregation of pre-nucleation clusters of particles larger than 500 microns. However, the large size of these particles may restrict the efficiency, scalability, and uniformity of current synthesis techniques. There is significant interest in developing new technologies for generating nano- and microparticles for biomedical applications. In this regard, a microfluidic-based biomineralization technology has been created, allowing for precise manipulation of reaction parameters through varied microfluidic settings. This method has successfully produced crystals ranging from 20 to 100 microns in size. Additionally, it facilitates the easy encapsulation of two model dyes: methylene blue (MB) and rose Bengal (RB). The proposed microfluidic synthesis technique presents a promising avenue for future research in particle production and drug delivery systems.

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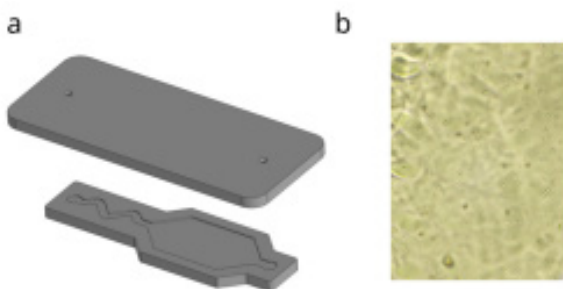
Aptamer-based microfluidic device for isolation of circulating tumor cells

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Prompt detection and treatment of oncological diseases is one of the most important problems of our time. One of the ways to solve it is the development of biosensors for diagnosing the disease at early stages by detecting circulating tumor cells. Here we present the design of a microfluidic device for capturing circulating tumor cells, a method for immobilizing aptamers on the surface of the chip reaction chamber, and an algorithm for controlling flows in microchannels. It was shown that the maximum efficiency of aptamer immobilization is achieved by treating the chip surface with a 50% aqueous-alcoholic NaOH solution. In addition, it was found that the greatest number of tumor cells of the MCF7 culture attached on the surface coated with aptamers at low flow rates of less than 2 min. It was noted that immobilized tumor cells are capable of being retained by aptamers at flow rates of up to 200 min



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Study of kinetics of liquid-liquid extraction of Am(III)/Eu(III) by N,O-donor ligands on a microfluidic setup

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One of the most studied and effective methods of separation of multicomponent systems such as high-level waste is solvent extraction. It is necessary to develop laboratory methods to compare and quantify extraction and mass transfer rates. Microfluidics has been used to quantitatively describe the kinetics of solvent extraction (see Figure 1).

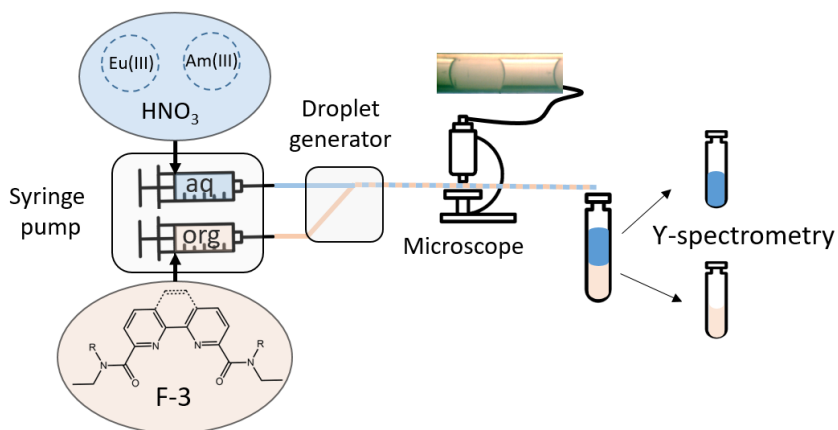


Fig 1 Microfluidic solvent extraction system

In this work, we quantitatively investigated the kinetics of extraction of Am(III)/Eu(III) pair for series of N,O-donor extractants and determined the rate constants of the process. The structure-kinetic properties relationship for this series was established and the influence of structural modifications on the extraction rate was shown.

We have shown how protonation affects the kinetics of extraction and ligand pre-organization. For this purpose, we determined Am(III)/Eu(III) mass transfer constants in different media in a system with BiPy-PhEt using a microfluidic setup.

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Microfluidic approach for fundamental studies of An(III) and Ln(III) liquid extraction kinetics

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Nuclear power is the most important source of CO₂-free energy. Its sustainable development is impossible without closing the nuclear-fuel cycle, which will lead to minimization of environmental risks and maximum recycling of resources. To achieve this, a spectrum of challenges must be addressed, one of which is the extraction of americium from high-level waste solution (HLW). Various extractants are being developed for this purpose. Promising extractants should satisfy several requirements, one of which is fast binding of metal cations in two-phase systems - aqueous and organic phases.

The targeted development of “fast” extractants at the moment is difficult due to the lack of relationship “extractant structure - extraction rate of metal cation”. And here, microfluidic extraction plays a special role for a detailed study of this kind.

The presentation will outline the problems arising in the development of extractants for rapid binding of metal cations under conditions of HLW solutions. The results of work carried out at the Department of Radiochemistry of Lomonosov Moscow State University will be presented.

Hydroformylation reactions under high pressure in microfluidic systems

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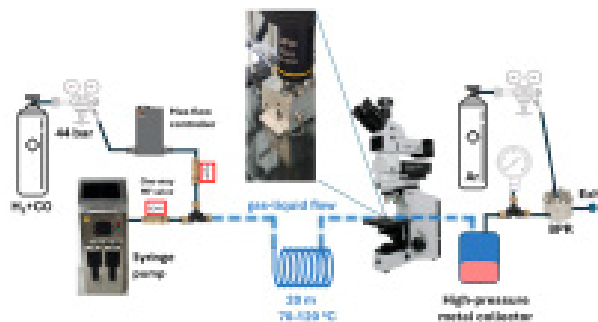
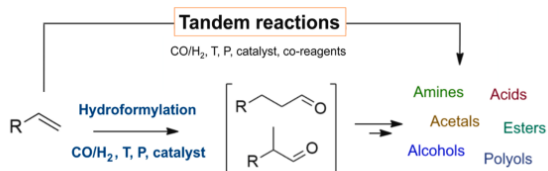
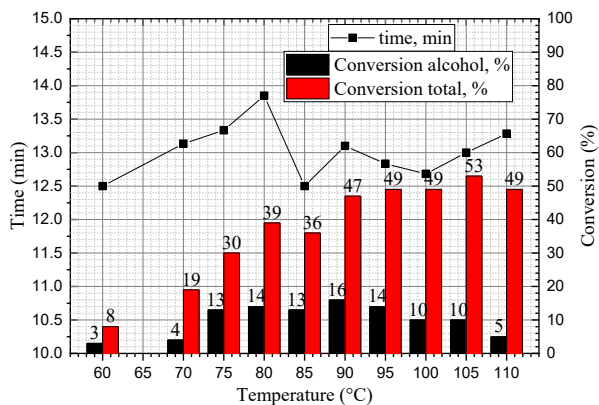
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Hydroformylation reactions using Rhodium (Rh) catalysts are widely used in industrial processes to produce aldehydes from alkenes. These reactions are typically conducted in autoclaves, where high pressures and elevated temperatures are required to maintain efficient gas-liquid mixing and maximize catalyst performance under these harsh conditions. This can be considered as a drawback. Microfluidics regime provides better results than batch already at lower pressure and residence time. The effect of different ligands on hexene hydroformylation was investigated at 120 oC and 42 bar using Rh complex in microfluidics and the conversion was measured using GLC techniques. Microfluidics showed higher conversion ~ 92% after 13 min using 18 m PEEK capillary. The same conversion was achieved only within 45 min in the autoclave. We observed tandem effect, producing alcohol subsequently from aldehydes and aldehydes from olefins in one step reaction. ~70% alcohol (heptanol) was obtained in 43 min at 50 bar and 90 oC. In conclusion, hydroformylation under high pressure in microfluidic systems offers a promising approach for efficient, selective chemical synthesis and could become essential to effective and environmentally friendly manufacturing processes.

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Development of hydrophobic resin and composite microfluidic devices based on it

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Abstract.

In this work, we apply an accurate and cost-effective DLP 3d-printing technique to fabricate droplet-based microfluidic chips [1]. We conducted a systematic study and showed how parameter tuning can change the surface properties of microfluidic devices. By selecting printing parameters, we were able to change the surface topology on a scale of 30-10 μm . Additional chemical modification of the printing material affects the surface roughness on a scale of 1-3 μm on the one hand and the surface wettability on the other. The combination of these two processes allows one printing method to simultaneously modify the surface geometry on two scales and achieve hydrophobic properties [2].

As a result, efficient droplet generators, delay lines, phase separators for droplet-based microfluidics have been obtained.

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The study was carried out with financial support from the Ministry of Science and Higher Education of the Russian Federation within the framework of the state assignment in the field of scientific activity no. FENW-2023-0019.

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Flow-through microfluidic synthesis of rare-earth doped scintillating nanoparticles with in situ control of X-ray induced optical luminescence and biodistribution study

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Thanks to high chemical and thermal stability, efficient energy transfer and tunable range of the photoemission fluoride-based nanoparticles doped with RE-elements are considered among the most promising materials for different applications including biomedicine technology. Conventional synthesis approach assumes thermal treatment at the temperature as high as 100-120° C along few hours, which makes the search for samples with optimized optical properties or particle size and morphologies time-consuming and resource demanding. Flow-through microfluidic synthesis of such scintillating nanoparticles is invoked to significantly optimize time and reagent consumption for multi-iteration search of the best synthesis conditions. Moreover, in our recent work we have demonstrated that not only SC NPs (BaGdF₅:Tb) but even composite materials for X-ray photodynamic therapy (XPDT) can be obtained within single-stage flow-through, by implementing an additional microfluidic reactor where the resulting reaction mixture conjugated with photosensitizer molecules without any intermediate stage such as drying, washing or supernatant removing from the initial particle solution. The possible obstacles and profits of such microfluidic synthesis for SC NPs and biodistribution studies of the composites on their basis will be discussed in the presentation.

Moreover, as more versatile system with higher structural and morphological diversity, we next consider the microfluidic synthesis of GdF₃ SC NPs doped with Ba and La in small amounts, which can be considered as a structure- and property-driven agents. The results are summarized and reported in the presentation.

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Development of a microfluidic system to investigate hemocompatibility and stability of coatings for blood pumping devices

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One of the most significant challenges in biotechnology, materials science, and medicine is to ascertain the capacity of diverse medical materials and devices to interact with biological systems in a manner that does not precipitate adverse effects, such as thrombosis and hemolysis [1]. The work proposes the design of a reversible microlab, a microfluidic chip, for a comprehensive investigation of the effects of engineered coatings on biological fluids, including blood. The research application of the device implies its operation in order to simulate *in vitro* actual contact conditions of the investigated materials with high shear stress fluid flow to determine the mechanical and hemocompatible properties of the materials. Due to the reversibility and microscale of the chip, it is possible to repeatedly investigate the behavior of coatings by operating with a small volume of liquid of 60 μ l, which ensures rational consumption of the biomaterials used. The connection of auxiliary microfluidic units enabled the regulation of fluid flow within the formed microchannel, thereby emulating a closed blood flow system with the requisite flow parameters.

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Real-Time Blob Detection with RGB Analysis in Video Feeds

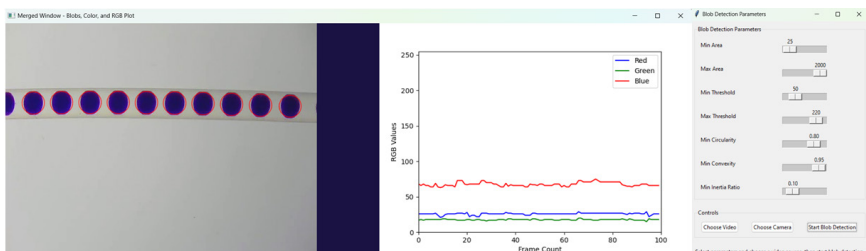
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The detection of blobs in real-time presents a significant challenge, particularly in environments where objects undergo dynamic changes in size, shape, and distribution, or when multiple blobs overlap[1]. This article aims to address these challenges by providing an adaptable and efficient solution, capable of handling complex and rapidly changing environments. The system offers a flexible, user-friendly interface that can be applied in fields such as object recognition, industrial monitoring, and fluid dynamics analysis. Real-time blob detection and analysis are crucial in various computer vision applications, including motion tracking, object detection, and pattern recognition[2]. The detection of droplets in situ presents a significant challenge, particularly in environments where the droplets are densely packed or undergo dynamic changes in size, shape, and distribution[3].

We propose a method for real-time blob detection with integrated RGB analysis, specifically designed for in situ applications where objects, such as droplets, are tracked and analyzed directly within their natural environment. The system efficiently processes video streams and dynamically tracks objects based on their shape, size, and color characteristics. By utilizing OpenCV for robust blob detection and a Tkinter-based graphical interface, users can adjust detection parameters in real time to optimize the detection process.



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Size distribution determination of colloidal particles and macromolecules in microfluidic systems.

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The progress in self-driving and smart laboratories is driven by novel analytical methods integrated in microfluidic systems for in situ feedback. A set of simple designs for microfluidic chip for DLP 3d-printing production that enables in situ DLS monitoring of ultra-low volumes of chemical and biological samples have been presented. Such method utilizes the signal backscattered light from the flow channel in microfluidics chip. However, a fluid motion affects the results of data analysis due to additional vector to Brownian motion. This artefact was overcome by sampling a tiny fraction of a primary flow with a low speed in a side channel.

A DLP 3d printer technology was used to manufacture microfluidic chips for in *situ* DLS measurements using fiber commercial DLS probe. The chip has a channel for sampling of tiny volumes from the reaction flow of the reaction mixture to perform DLS measurements as in static conditions during undisturbed flow in the main channel. Using such approach DLS measurements could be directly performed during synthesis/production without additional calibration for the flow speed velocity. The capability of in *situ* hydrodynamic size determination is a promising solution to incorporate DLS into high-throughput screening systems or production lines in chemical, food, and bio-medical industry.

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Numerical and experimental approach to the study of single-phase and multiphase flows in the elements of microfluidic devices.

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Microfluidics is a new emerging interdisciplinary science of the 21st century, where fluid mechanics comes into contact with many fields of physics, chemistry and biology. This work is focused on the application of computational and experimental approaches to the study of the features of single-phase and multiphase flows in several configurations of microchannels of complex internal structure. Flow in channels of this geometry is often found in heat exchangers, as a part of functional elements of microfluidic devices applied in medicine, chemical engineering, oil and gas industry, etc.

The developed numerical approach is based on the BEM accelerated both via the fast multipole method (FMM), and heterogeneous computing architecture (multicore CPUs and graphics processors). The experimental part is based on modern methods with the use of high-speed cameras, methods of optical microscopy (including fluorescent), technology for the construction of integrated micro-setups based on microfluidic devices manufactured using the "lab-on-a-chip" technology. This work presents the results of application of the described approaches to study the flow and dynamics of disperse systems in micromodels of porous media with several porosity scales, in microchannels with contraction-expansion array, with deterministic lateral displacement of elements, etc.

The proposed approach and the obtained results can be used to investigate practically significant problems related to the study and development of methods of influence on single- and multiphase flows in functional elements of microfluidic devices.

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Real-time diagnostics of catalytic reaction products in microfluidic systems

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The research introduces an innovative heterophase Pt/ethylene glycol catalytic system for hydrosilylation reaction, which is integrated into a microfluidic platform to enhance efficiency and address economic and environmental concerns associated with traditional Pt catalysis. The microfluidic regime improves mass and heat transfer, creating a stable environment for the reaction and offering advantages over batch processing methods. In situ Raman spectroscopy is utilized for continuous, real-time monitoring of the reaction, enabling automated conversion analysis and faster, more accurate data collection. The microfluidic reactor's components are designed using both commercial units and 3D printing technology, allowing for customization and cost-effective production. This work marks the first implementation of a semi-automatic recyclization device for heterophase catalytic processes, presenting a scalable solution for the sustainable and automated production of organosilanes in the chemical industry.

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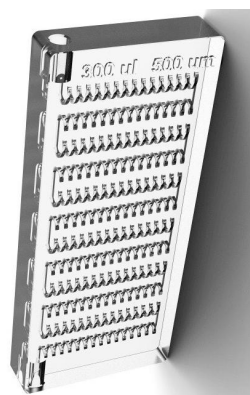
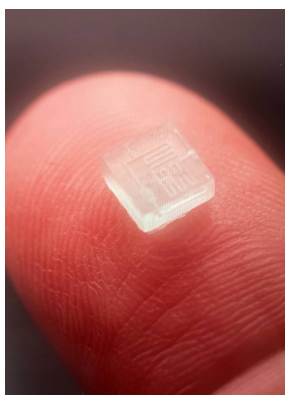
Development of microfluidic systems via 3d printing additive DLP approach: experience and case studies

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Automatized flow systems overcome the difficulties inherent for the conventional batch approaches. Microfluidic systems represent a good alternative for the high throughput data collection. Elements of microfluidic systems created by 3D printing offer numerous advantages, such as rapid manufacturing, low cost, and the ability to create complex 3D channel topologies. Their parameters and performance can be quickly adjusted by editing the model loaded into the printer. The recent advances in 3D-printing made complex topologies in microfluidic devices cheaper and easily customizable. In this work we present 3D-printed systems for different chemical and biomedical applications including monodisperse droplet generation, noble metal nanoparticle synthesis, protein crystallization.



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Targeted Isolation of Circulating tumor cells(CTC) on Aptamers-functionalized Biofilm Integrated inside Microfluidic chip

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Circulating tumor cells (CTCs) can be isolated through either active or passive methods. Active techniques utilize external fields such as electric, magnetic, acoustic, and optical forces to facilitate cell separation. In contrast, passive methods rely on channel designs, inherent hydrodynamic forces, and steric hindrances to manage cell movement. However, isolating biological materials with complex compositions, like whole blood that contains various cell types, poses challenges for single-module microfluidic devices. Recently, integrated microfluidic devices that combine both passive and active elements have gained popularity as a label-free enrichment technique for CTCs due to their numerous advantages, including high sensitivity and efficiency in processing multiple target cells.

In this context, we developed, described, tested, and integrated a hybrid Chitinous (CS) membrane onto a prototype microfluidic chip to enhance biocompatibility and facilitate CTC research. This membrane is approximately 10 μm thick and can be modified for porosity while being sufficiently biocompatible to mimic a basement membrane. The design of the sample chip was modelled to identify optimal fluidic conditions for utilizing the membrane in future studies. To extract target tumor cells and clusters from whole blood, an integrated biofilm was previously modified with two distinct targeting molecules: folate receptor-targeting FA and breast cancer (Bc) targeting Aptamer. The biofilm's adherence allowed for controlled and targeted isolation of CTCs based on flow velocity, achieving a purity of 90% for tumor cell clusters while maintaining over 95% cell viability. The integration of the proposed membrane into microfluidic devices represents an innovative approach that can be adapted into a customizable platform

suitable for various applications, including drug delivery, organ-on-chip systems, and anticancer therapies.

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Microfluidic system for screening of gold nanoparticle synthesis parameters

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This work describes high throughput microfluidic screening of reagents combination for synthesis gold nanoparticles with UV-Vis spectral diagnostic. The system was adapted for automatic work protocol. System performed screening into 27 synthesis parameters combinations for one hour and collected more than 200 thousand absorptions spectra.

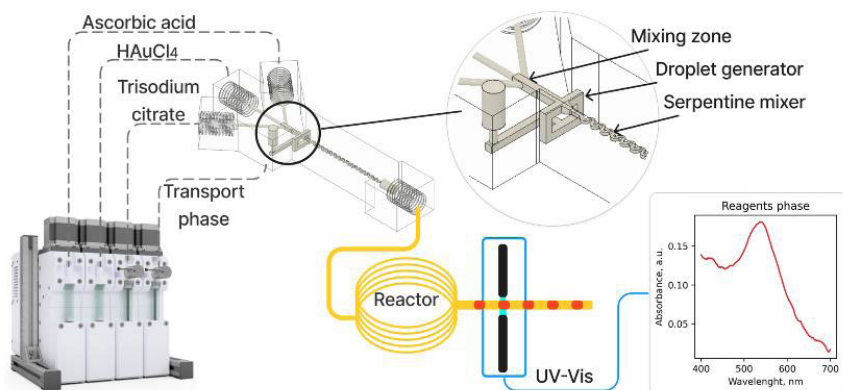


Fig 1. Scheme of the experiment

Synthesis method based on the modified Turkevich method [1], which utilizes trisodium citrate and ascorbic acid, due to gold particles within 15-150 nm range can be synthesized. Diagnostics was based on investigation of localized surface plasmon resonance (LSPR) with a strong absorbance maximum in the visible light region [2].

For separating spectra we develop, specific algorithm was based on the differences between reagent and transport phase and on the statistical analysis. Spectra belonging to one set of parameters were averaged and multiple descriptors were calculated from them.

The Extra Trees machine learning algorithm was trained on a dataset comprising the descriptors and reagent flow rates. For example, the intensity of LSPR provides a qualitative measure of colloidal mixture homogeneity. Higher intensity of the peak at similar concentration indicates narrower size distribution of nanoparticles.

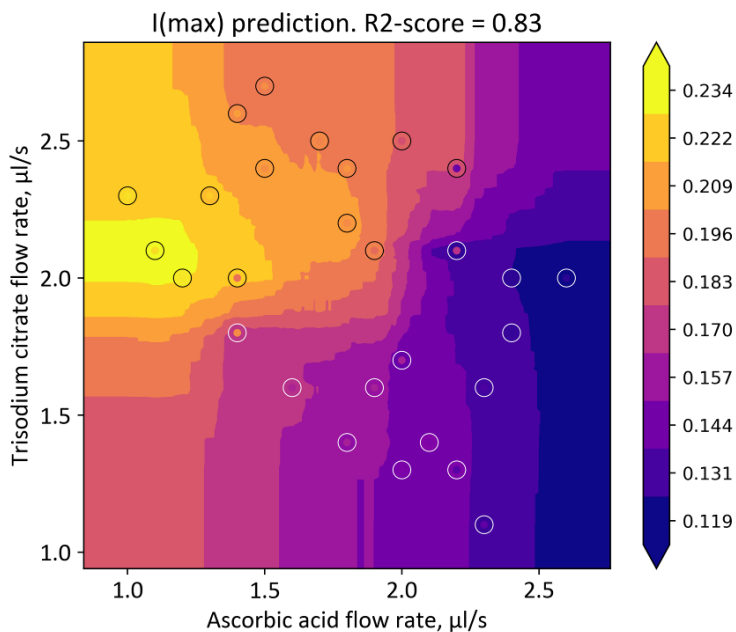


Fig 2. Prediction map of maximum intensity of plasmon resonance peak

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