ELKIN 2026 – Poster abstracts

1 Fatemeh Hashemifar - In-Situ Bubble Analysis in Alkaline Electrolysis

Fatemeh Hashemifar, Jeff Wood, Rob Lammertink

In zero-gap alkaline water electrolysis (AWE) bubbles can cover the electrode surface, increasing overpotential and impacting efficiency. This research examines hydrogen bubble nucleation and detachment dynamics in confined spaces, where microscale phenomena influence mass transport and electric field distributions. Understanding these dynamics is essential for optimizing hydrogen output and reducing energy losses.

2 Sungyeol Kwak - Ionic-Conductance-Enhanced Nanofluidic Memristor Enabling Low-Voltage Neuromorphic Computing

Sungyeol Kwak, Dong-yup Lee, Hyomin Lee, Hayoung Yun, Jeong-Yun Sun and Sung Jae Kim

Fluid memristors have emerged as a promising class of neuromorphic devices by emulating ion-mediated signal processing in biological synapses. However, most previously reported memristors operate at relatively high voltages (≥100 mV) and rely on non-biocompatible ionic species such as Ag^+, which limits their suitability for low-power neuromorphic systems and direct interfacing with bio-potential-level signals. Here, we present a nanofluidic memristor based on a three-dimensional asymmetric architecture integrated with nanoporous hydrogel PN junctions. By leveraging coupled electric, diffusive, and electrohydrodynamic ion transport mechanisms, the device exhibits pronounced hysteresis, nonlinear memory characteristics, and synaptic plasticity under genuine bio-potential-level stimulation. The hydrogel-based architecture further provides intrinsic biocompatibility while enabling low-energy operation. The proposed device demonstrates (i) synaptic plasticity at voltages of only a few millivolts, (ii) reliable responses to low-amplitude input signals down to 100 μV, and (iii) fast neuromorphic dynamics under sub-microsecond pulse excitation. These results establish the nanofluidic memristor as a viable platform for low-voltage neuromorphic computing and suggest a pathway toward biocompatible and energy-efficient interface systems beyond conventional solid-state memristors.

3 Johannes Schenk - Ammonium Removal by Membrane Capacitive Deionization: Effects of Voltage, Current, and Flow on Removal Efficiency, Water Recovery, and Energy Demand

Johannes Schenk, Nick Schäuble, Anu Suresh, Jan Hoinkis

Membrane capacitive deionization (MCDI) is a promising electrochemical technology for the selective removal and recovery of nutrients from aqueous streams, including municipal and agricultural wastewater as well as groundwater. In this context, ammonium (NH_4^+) removal is of particular relevance, as it helps prevent environmental impacts such as eutrophication [1] and may be required to meet drinking water quality standards [2]. In various water treatment applications, MCDI has been reported to achieve high water recovery and energy efficiency, partly due to its operation at low pressures [3]. However, maintaining these advantages becomes challenging when targeting high ion removal efficiencies.

In this study, the performance of an MCDI system for NH_4^+ removal was investigated over

a broad range of operating conditions, with a focus on achieving high removal while preserving favorable energy and recovery metrics. A synthetic feed solution with an NH_4^+ concentration of 500 mg/L was used. Experimental parameters included flow rates between 15 and 54 L/h, applied cell voltages of 1.5 to 1.9 V, current densities between 12 and 20 A/m², and adsorption–desorption cycle times of up to 400 s. All experiments were conducted using an industrial MCDI module with an electrode area of 3 m². NH_4^+ removal efficiencies exceeding 99% were achieved under appropriate electrical and hydraulic regimes. In addition to removal efficiency, water recovery and specific energy consumption (SEC) were calculated to enable a comprehensive assessment of process performance. The results reveal trade-offs between throughput, energy demand, and recovery metrics, while identifying operating windows in which high NH_4^+ removal can be maintained alongside acceptable water recovery and SEC.
The poster presents the experimental setup and measurement strategy, as well as an analysis of how operating parameters can be optimized to enhance water recovery and reduce SEC without significantly compromising NH_4^+ removal efficiency. Ongoing experiments further expand the dataset and are included in the poster, enabling a more detailed analysis of the operational regimes. These findings support the potential of MCDI for applications with high ion removal requirements and provide guidance for performance optimization in future scale-up and application-oriented studies.

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4 Sinwook Park - Printed-Circuit-Board-Integrated Iontronic Circuits for Ionic Logic Gate Computation and Memory-Based Signal Processing

Sinwook Park, Noa Edri Fraiman, Roy Nesher, Alexander Fish, Gilad Yossifon

Interfacing iontronic components with printed circuit board (PCB) platforms offers a scalable pathway for realizing iontronic circuits composed of multiple addressable elements, enabling future bio-compatible computing and sensing systems. In this work, we demonstrate the implementation of iontronic circuits on PCB substrates, beginning with integrated ionic logic gates—including AND, OR, and multi-gate combinations—constructed from bipolar polyelectrolyte diodes [1]. We examine circuit addressability using PCB-embedded electrodes in comparison with the conventional use of external electrodes. While external electrodes (e.g. Ag/AgCl wires) provide stable reference potentials for baseline characterization, PCB-embedded electrodes enable miniaturized, multi-channel routing essential for on-chip integration and scalability.
Furthermore, we investigate history-dependent signal processing using polyelectrolyte-based memristors, demonstrating a platform extendable to biomimetic dendritic architectures [2]. By coupling volatile memristors with distinct time constants—tuned via geometric scaling and neutral hydrogel spacer length [3]—we realize synapse-like units capable of concurrent short-term and long-term potentiation and depression (STP/LTP). These behaviors arise from induced ionic concentration polarization (ICP)-based signal processing effects[4]. This architecture supports inherent on-chip communication

between iontronic components, offering a promising route toward fully fluidically interconnected iontronic circuits.

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5 Samira Aliasghari - Electrosorption of Short-Chain PFAS using innovative colloidal activated carbon/graphene composite electrodes

Samira Aliasghari, Navid Saeidi, Ali Shaygan Nia, Xiliang Feng, Anett Georgi

Per- and polyfluoroalkyl substances (PFAS) are a large class of synthetic organofluorines widely used for their thermal stability and surfactant properties. Their exceptional persistence, mobility, and potential toxicity have led to increasing concern in drinking-water treatment. Short- and ultra-short-chain PFAS are highly mobile in water and exhibit low affinity for conventional adsorbents, leading to fast breakthroughs on granular activated carbon (GAC) filters and weak retention by many pressure-driven membranes. The same properties cause environmental persistence and create compliance risks with the EU Drinking Water Directive limits that became mandatory in 2026 that became mandatory since 2026 (0.1 µg/L sum of 20 PFAS or 0.5 µg/L PFAS total [1]. This “treatment gap” motivates the evaluation of active, electrically driven separation processes that can enhance removal of short-chain and ultra-short-chain PFAS and concentrate them into small volumes for subsequent management. Electrosorption, which is defined asthe field-driven, reversible uptake of ions at polarized electrodes, offers a promising path to address this challenge. By applying a positive potential to an electrode, negatively charged PFAS species (at neutral pH, typically carboxylate or sulfonate anions) are adsorbed on the electrode due to enhanced electrostatic attraction, together with other possible mechanism such as hydrophobic effects and van-der-Waals interactions [2]. While switching potential to negative values releases the PFAS anions loaded on the electrode to water.
This study investigates the electrosorptive removal of short- and ultra-short-chain PFAS from water using stable porous carbon-based composite electrodes to enhance: 1) electrosoption modulity and 2) electrosorption kinetics. Stable porous carbon-based electrodes were prepared using colloidal activated carbon (CAC, mean particle diameter = 1 µm) alone and in combination with amino-functionalized graphene. CAC provided high specific surface area and rapid mass-transfer pathways for PFAS uptake, while incorporation of amino-functionalized graphene enhanced electronic conductivity and capacitance and introduced positively charged surface functionalities at circumneutral pH due to the functional groups.
Electrosorption experiments with perfluorobutanoic acid (PFBA, C_0 = 100 µg L^{-1}) achieved distribution coefficients (Kd) of up to 4000 L kg^{-1} at an applied potential of +600 mV vs. Ag/AgCl. Reversal of the applied potential enabled almost complete desorption of PFBA with Kd ≤ 80 L kg^{-1} at potential -400 mV vs. Ag/AgCl, confirming the fully reversible and electrically controlled nature of the electrosorption process. Systematic variation of the graphene:CAC ratio further demonstrated that amine functionalities enhanced electrostatic attraction of anionic PFAS, resulting in improved electrosoption coefficient, faster electrosorption kinetics, and increased cycling stability compared to CAC electrodes.

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6 Boaz Kuizenga - Enhancing Selectivity in Electrochemical Alcohol Oxidation Through Reference Electrode Integration in a Microflow Reactor

Boaz Kuizenga, Simon Kuhn

Aldehydes are essential intermediates in the chemical and pharmaceutical industry(1). While most studies focus on secondary alcohols, selective oxidation of primary alcohols to aldehydes remains underexplored(2). Cyclic voltammetry indicates that controlling the anode potential can suppress over oxidation(3). This work investigates how the use and placement of a reference electrode in a flow reactor can improve aldehyde selectivity by enabling precise potential control.

A custom microflow reactor equipped with platinum coated titanium electrodes (active area: 15.3 cm²) and 9 different Ag/AgCl reference electrode positions (relative to the flow field) will be operated under galvanostatic and potentiostatic conditions. It will be assessed how fixed, lower potentials and key reactor design parameters — specifically reference electrode position, flow field geometry, and electrolyte composition — influence conversion and product selectivity.

Detailed experimental data will be presented to showcase the increase in selectivity towards the aldehyde when controlling the anode potential (approximately 0.9V vs NHE). Furthermore, we investigate the effect of the reference electrode position, as it can potentially influence the accuracy of the potential measurement, which in turn influences the conversion. Thus, we will provide guidelines for the integration of reference electrodes in micro-scale electrochemical reactors.

This study provides insight into primary alcohol oxidation mechanisms and highlights design considerations for improved selectivity control in electrochemical flow reactors.

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7 Tina Đukić - Improved Durability of Pt-nanoalloy-based Oxygen Reduction Reaction Electrocatalysts for Low-temperature Fuel Cells: Tuning the Intrinsic Properties

Tina Đukić, Iva Klofutar, Ante Matošin, Leonard Jean Moriau, Matija Gatalo, Nejc Hodnik*

The development of Pt nanoalloys as oxygen reduction reaction (ORR) electrocatalysts for fuel cells has progressed significantly in recent decades. However, to make the Pt nanoalloys superior compared to the still most commonly used Pt in the fuel cell market, it is crucial to solve a key issue – to enable a long-term durability of these electrocatalytic systems under aggressive conditions of a proton exchange membrane fuel cell (PEMFC). Namely, the continuous leaching of a less noble 3d-transition alloying element (such as Co) from the Pt-nanoalloy-based electrocatalyst, and the consequent contamination of the ionomer of cathode catalyst layer as well as the proton exchange membrane with dissolved alloying-element species, represent a serious problem for the longevity of the PEMFCs, which is particularly pronounced in the heavy-duty vehicle applications. Therefore, improving the durability of Pt nanoalloys must be addressed.[1]

In this regard, in previous research we have shown how playing with potential/voltage limits can be used as an approach to extend the lifetime of Pt nanoalloys under operating conditions of the PEMFC.[2,3] On the other hand, here we will focus on tuning the intrinsic properties of Pt nanoalloys as a tool for improving both activity and durability of these electrocatalysts. In particular, the effect of the atomic ratio of Pt to Co on the stability behavior of the carbon-supported Pt-Co nanoalloys has been investigated. For research purposes, four in-house designed electrocatalysts (Pt2.69Co, Pt1.23Co, Pt1.19Co and Pt0.81Co) have been tested using two in-house designed and previously widely described methodologies: (i) high-temperature disc electrode (HT-DE) methodology,[1–3] which enabled the performance of accelerated degradation tests (ADTs), composed of 10,000 trapezoidal wave cycles between 0.6 and 0.95 VRHE with a 3 s hold at each potential limit, in a 0.1 M HClO4 electrolyte at 60 °C, thus allowing a simulation of close-to-real PEMFC conditions, and (ii) electrochemical flow cell coupled to an inductively coupled plasma mass spectrometry (EFC-ICP-MS),[1–4] which enabled in situ metal dissolution measurements. Interestingly, whereas enriching the Pt-Co-based electrocatalyst with Co was expected to increase the intrinsic activity towards ORR, there appears to be a threshold Co level beyond which the kinetic properties depend on another intrinsic factor, particularly the crystal structure. Namely, the presence of the L10-PtCo (P4/mmm) tetragonal intermetallic phase in Pt1.19Co has shown to benefit the ORR activity not only at the beginning of the electrocatalyst lifetime but also after the performed ADT, due to the highest retention of Co, and consequently the highest retention of the strain effect, among all the investigated electrocatalysts. Therefore, adjusting the Pt-to-Co ratio can be used as a main approach in the electrocatalyst design for achieving a compromise in the activity-stability relationship.

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8 Albert Liu - Modular Electrochemical Sensing via In Situ Reduced Carbon Quantum Dot–Nanotube Molecular Hybrids

*Jihpeng Suna, Jack Johnstonb, Adam Robertsa, Albert Tianxiang Liua,c,d,e**

Electrochemical sensing is a promising route to non-invasive, point-of-care health monitoring, yet practical multiplexing remains limited by electrode materials that cannot simultaneously deliver high conductivity, high densities of electrochemically active sites, and modular surface chemistry for targeted analyte specificity. Here we introduce a hybrid nanocarbon architecture that decouples charge transport from surface reactivity by grafting oxygen-rich carbon quantum dots (CQDs) as a chemically active “skin” onto a conductive multiwalled carbon nanotube (CNT) scaffold (CQD@CNT), then applying in situ electrochemical reduction to strengthen interfacial electronic coupling while preserving functional groups that promote analyte adsorption and catalysis. By systematically tuning the reduction potential, we identify an optimal regime that maximizes CQD–CNT interfacial coupling and charge transport while avoiding over-reduction that compromises sensor activity. Spectroscopic and electrochemical characterization reveals partial deoxygenation and restoration of conjugation within the hybrid material, increased electrochemically active surface area, and a pronounced decrease in charge-transfer resistance after in situ reduction. Using differential pulse voltammetry, the reduced molecular hybrids exhibit enhanced sensitivity toward uric acid, and support multiplexed detection of uric acid, dopamine, and ascorbic acid within a single voltametric scan. Sensor modularity is further demonstrated by covalently grafting 18-crown-6 to CQDs to enable Pb^{2+} detection via anodic stripping voltammetry on unchanged CNT scaffolds, illustrating how molecular recognition can be integrated without compromising electron transport. Our work establishes in situ electrochemcial reduction as a scalable, post-fabrication strategy to address the conductivity–activity trade-off in electrochemical sensing and provides a generalizable CQD@CNT platform for multiplexed biosensing and environmental monitoring.

9 Cloë Berkien - Separator development for alkaline water electrolysis

Water can be split into hydrogen and oxygen gas upon charging an electrochemical cell, known as a water electrolyzer. This generated green hydrogen is unlike hydrogen produced from fossil fuels, as its production does not emit greenhouse gases when coupled to a renewable energy source. Hydrogen is of significant relevance for many chemical industries, and in addition, can serve as an energy carrier by storing electrical energy in the form of chemical energy, which can be converted back into electrical energy in a fuel cell when required. This is especially valuable given the continuously increasing contribution of renewable energy sources, such as wind and solar, which are weather dependent and therefore fluctuate accordingly. Storing surplus energy, for instance in green hydrogen, enables a more constant energy supply by bridging periods of reduced renewable energy generation.
There are various technologies that enable the generation of hydrogen through water electrolysis, of which alkaline water electrolysis is the most mature due to its relatively cheaper and more robust materials. In this technology, the electrolyte separating the two electrodes is of a highly alkaline pH to enhance conductivity and the redox reactions at the electrodes. A porous separator is placed between the two electrodes to separate the

produced gases, whilst allowing electrolyte infiltration for ionic transport. However, despite its relative maturity, the operation of alkaline water electrolysis is still limited by high resistances within the electrolyzer cell, with transport limitations mostly occurring in the separator. In addition, the produced gases are not always sufficiently separated to maintain safe and continuous operation conditions.
The separator's performance is dependent on a trade-off between conductivity and gas crossover. Improving one often worsens the other. Therefore, this project focuses on finding the right chemical composition and manufacturing method to manipulate transport processes in the electrolyzer, in turn allowing for optimal performance. The goal is to fabricate a sustainable separator that allows for improved conductivity, limits the mixing of hydrogen and oxygen, and remains chemically and physically stable in highly alkaline and heated environments.

10 Paul Takhistov - Coupled Electrokinetic and Electrodiffusion Transport near Dissolving Anodes: Protein-Induced Heterogeneous Crystallization of Metal Nanoparticles

Paul Takhistov, Michael Shen

Application of an electric field to protein suspensions results in electrophoretic concentration of proteins near the anode, forming a highly viscous interfacial layer rather than a solid deposit or self-assembled film. This layer forms adjacent to an electroactive anode that simultaneously dissolves, releasing metal ions into the same region. This work describes the process as a coupled electrokinetic–electrodiffusion transport problem. Protein transport toward the anode is dominated by electrophoretic drift, while diffusion is negligible due to low particle mobility and strong concentration-dependent viscosity. In parallel, metal ions generated at the dissolving anode are transported by electrodiffusion into the protein-rich viscous layer. The concentrated protein phase acts as a reactive precursor and heterogeneous nucleation medium, promoting crystallization of metal nanoparticles with characteristic sizes in the 20–100 nm range. No salt addition, antisolvent, or chemical precipitation step is required: nanoparticle formation arises solely from the interaction between electrophoretic protein concentration and ion flux from the electroactive interface. The resulting protein–metal nanocomposite forms in situ within the viscous interfacial layer. A transport-based analysis identifies the roles of electric field strength, electrophoretic Péclet number, and anodic dissolution rate in controlling layer growth and nanoparticle formation.

11 Wenge Huang - Stability Analysis of Oscillating Hydrogen Bubbles on Microelectrodes

Hydrogen bubble dynamics critically influence transport efficiency, electrode performance, and energy conversion in microelectrolysis systems. Despite extensive studies on bubble growth and detachment, the stability characteristics of hydrogen bubbles under coupled electrochemical, capillary, and hydrodynamic effects remain insufficiently resolved. Here, we perform a numerical stability analysis of hydrogen bubbles nucleated on microstructured electrodes using high-fidelity interface-resolving simulations. The governing equations couple incompressible Navier–Stokes dynamics with electrochemically driven gas generation and surface tension effects. A linear stability framework is established to quantify the onset of interfacial deformation under competing influences of capillarity, buoyancy, viscous stresses, and electric-field-induced body forces. We systematically investigate the role of electrode microgeometry, contact line conditions, gas production rate, and electrolyte properties on bubble shape stability and detachment thresholds. Our results reveal distinct instability modes governed by a

balance between capillary confinement and electrohydrodynamic forcing. Microstructural confinement modifies the critical Bond number and shifts the dominant instability wavelength, thereby altering the detachment pathway. Furthermore, we identify a scaling relation linking gas generation flux to interfacial growth rate and stability margin. These findings provide mechanistic insight into hydrogen bubble retention and release in microelectrolysis, offering design guidelines for optimizing gas removal and enhancing electrochemical efficiency.

12 Jihee Park - In-Operando Analysis of Nanoelectrokinetic Phenomena Governing Dendrite Growth at Metal Anode Interfaces

Jihee Park, Donghyun Kim, Prof. Sung Jae Kim

Dendrite growth on metal anodes is closely associated with ion depletion and concentration polarization at the anode–electrolyte interface during electrochemical charging. When the rate of metal ion transport to the electrode surface cannot keep pace with the electrochemical deposition rate, ion depletion develops near the interface, leading to interfacial instability and directional dendrite growth. Although highly concentrated electrolytes have been proposed to mitigate the transport limitations, the actual electrode–electrolyte interface is governed by coupled nanoelectrokinetic phenomena, including steep ion concentration polarization and the formation of strong interfacial electric fields, which further accelerate dendrite growth. In this work, we develop a transparent microfluidic platform for in-operando investigation of the electrode–electrolyte interface, enabling real-time visualization and quantitative analysis of nanoelectrokinetic phenomena accompanying dendrite growth. Fluorescent probes are employed to map interfacial concentration and flow fields, while micrometer-scale electrochemical probes are used to precisely quantify local electric fields and ion depletion behavior. This approach provides a new experimental framework for elucidating the nanoelectrokinetic mechanisms governing dendrite growth at metal anode interfaces.

13 Tibor Pálszegi - Electrokinetically Steered Pattern-Forming Textiles (ES-PFTs)

Electrochromic smart textiles provide a scalable platform for adaptive garments and soft electrochemical devices. While AeroSkin represents a well-established benchmark in which applied voltage drives local electrochromic switching in a pixel-like manner, we propose a complementary paradigm: Electrokinetically Steered Pattern-Forming Textiles (ES-PFTs). In ES-PFTs, spatial optical textures arise autonomously through reaction–diffusion electrochromic dynamics and are subsequently steered by boundary-driven electric forcing, enabling continuous-field control without pixel addressing.
Autonomous pattern generation is modeled using a Gray–Scott-type reaction–diffusion system with two minimal state variables, which produces spatial textures through intrinsic instability and wavelength selection.
Electrokinetic steering is introduced via a spatially distributed, time-dependent potential field, computed in two complementary forms: (i) a PDE-based potential formulation for the electrolyte/ion-gel sheet and (ii) a Transmission Line Model (TLM) / RC-sheet network representation capturing lateral current redistribution and distributed interfacial capacitance under phase-driven electrode patches. Electrode symmetry and phase-coded AC forcing determine macroscopic motion modes, including oscillatory shear (2 electrodes), traveling drift (3 electrodes), and controlled rotation (4 electrodes), with CW/CCW reversal controlled by phase ordering. This combined Gray–Scott + PDE/TLM electrokinetic framework supports low-wiring smart fabrics that behave as steerable continuous materials rather than display-like arrays.

14 Manish Chauhan - Unveiling the Role of Platinum and Graphite Counter Electrodes in Water Splitting with CVD-Grown Iron and Nickel Oxide Anchored Carbon Nanofibers

Manish Chauhan (Presenter), Pradip Kumar (Corresponding), Shiv Singh (Corresponding)

Efficient and durable electrocatalyst is the vital concern for top-tier sustainable green hydrogen production. In this study, chemical vapour deposition (CVD) grown iron and nickel oxide- carbon nanofibers (FeO-CNF and NiO-CNF) were thoroughly evaluated for water-splitting undergoing hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline medium. The CVD-induced uniform & continuous tip-growth and vertical alignment of the CNFs significantly enhanced charge-transfer kinetics. Additionally, the electrochemical system was assessed linking two different and equally prevalent counter electrodes, platinum and graphite. As a result, FeO-CNF favours HER activity, delivering overpotentials of 380 and 560 mV at 10 mA/cm2 with Pt and graphite, respectively, outperforming NiO-CNF. In contrast, NiO-CNF demonstrated enhanced OER performance, with overpotentials of 420 mV with Pt and 445 mV with graphite at 10 mA/cm2, approaching those of benchmark RuO2 catalysts. Further, an alkaline water electrolyzer was also tested, utilizing the two concerned electrocatalysts. To improve ion migration, the same catalyst materials were used at both the anode and cathode, and electrochemical measurements were conducted in 1 M KOH solution. Under these conditions, NiO-CNF exhibited greater stability than FeO-CNF. Specifically, the cell voltage for FeO-CNF decreased from 1.6 to 1.5 V after 24 h, whereas the voltage increased from 2.0 to 2.5 V after 24 h in the case of NiO-CNF. Overall, CVD-grown FeO- and NiO-CNFs exhibit complementary electrocatalytic behaviour, underscoring their potential as efficient bifunctional materials for alkaline water-splitting applications, and in-turn, inferring Pt as better counter electrode for HER while graphite favouring OER.

15 Yanbo Xie - Negative Differential Flow Resistance in Reverse Osmosis

Fan Li, Ziheng Wang, Yanbo Xie

Reverse osmosis (RO) is an efficient desalination approach, but the widely used solution-diffusion model was challenged for failing to explain field-dependent permeabilities, particularly when the continuum theory may break down in Ångström scale. Here we developed a non-equilibrium statistical theory, supported by molecular dynamics simulations that captures the field-dependent water and ion permeabilities through a single Ångström-scale channel. Surprisingly, our simulation reveals a counterintuitive negative differential flow resistance (NDFR) effect, where the flow velocity decreases with increasing pressure. This phenomenon arises from ion trapping at the nanotube entrance, caused by dielectric and dehydration barriers and hydrodynamic friction. The NDFR effect significantly reduces water permeability and may be a predominant factor constraining the selectivity-permeability trade-off in RO. Our statistical theory is based on a bidirectional escape framework that predicts the pressure- and size-dependent permeabilities and explains the NDFR effect. Our findings offer molecular-level insights into RO and can be extended to broader transport phenomena in confined systems.

16 Duc N. Dinh - Standardized, Scale-Invariant Performance Benchmarking of Membrane Capacitive Deionization Toward Industrial-Scale System Design

Duc Ngoc Dinh, Edgardo Cañas Kurz, Ulrich Hellriegel, Jan Hoinkis

Membrane capacitive deionization (MCDI) is governed by coupled electrokinetic, transport, and capacitive processes. However, the absence of standardized benchmarking methodologies has limited meaningful comparison across module designs, operating conditions, and scales. This discrepancy has impeded the translation of laboratory-scale advancements into reliable industrial system design. This study proposes a standardized performance benchmarking and normalization framework. This framework is designed to capture the intrinsic electrokinetic behavior of MCDI modules under scale-relevant operating conditions.
The framework delineates a set of key performance indicators (KPI) that are grounded in physical principles. These KPIs encompass metrics such as total salt adsorption capacity, effective capacitance, and characteristic time constants. The utilization of these KPIs facilitates the evaluation of module output efficiency. A systematic normalization methodology is introduced to decouple intrinsic performance from extrinsic variables. These extrinsic variables include geometric scaling, applied current density, hydraulic residence time, and feed salinity. This facilitates direct, quantitative comparison across module sizes, architectures, and operational windows.
Beyond single-cycle evaluation, the proposed protocol incorporates cycle-resolved performance metrics for repeated operation, allowing assessment of dynamic electrokinetic response, capacitance evolution, and efficiency degradation under realistic cycling conditions. A thorough, long-term, multi-cycle analysis has been conducted, revealing the occurrence of performance drift and capacity fade phenomena. These phenomena are not captured by conventional single-cycle benchmarks.
By establishing a reproducible and scale-independent benchmarking protocol, this work establishes a quantitative foundation for module-to-module comparison, predictive stack sizing, and control strategy development. The proposed framework signifies a pivotal advancement in the direction of standardized performance assessment tools, which are imperative for the design, optimization, and accelerated deployment of systems.

17 Senne Fransen - Simulating dipolophoresis with automatic differentiation

Senne Fransen, Willem Van Roy, Maarten Rosmeulen

Under the weak external field approximation, electrophoresis (EP), dielectrophoresis (DEP), and electrokinetic effects such as induced charge electrophoresis (ICEP) or concentration polarization electrophoresis (CPEP) can be analyzed with 1st (EP) and 2nd order (DEP, ICEP, CPEP) perturbation theory. The approach typically found in literature performs an analytical perturbation expansion in terms of the external electric field strength as a first step, followed by implementing the model equations, order-by-order, in a finite element solver (e.g., [1]). Since the model equations are solved numerically anyway, we previously showed that it is equally valid to first discretize the model equations and then perform the perturbation analysis [2]. This approach is attractive, as the discretization-first approach allows for clearer generalizations to more complex cases: It programmatically only requires the model residuals and a so-called Jacobian matrix. In addition, irrespective of which approach is taken, the Jacobian matrix is anyway needed for finite-element solvers and efficient construction methods have been developed [3]. Therefore, if one has access to the residuals and Jacobian, any second-order perturbation problem can be solved with relative ease. To illustrate the generality of the approach, we concretely present a Python implementation that allows us to calculate the "dipolophoretic [4]" response of a composite core-shell nanoparticle with non-negligible double layer in a buffered electrolyte containing any number of ionic species. It also becomes straightforward to implement much more advanced models of the double layer (for example, see [5]) that are too elaborate to implement using conventional approaches.

The discretize-first approach therefore opens new possibilities to simulate realistic cases closer to applications beyond idealized model particles, binary electrolytes, and geometries.

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18 Renske Groen - Modelling the removal of ionic species from multicomponent feedwater in an electrodialysis system.

This research focuses on developing a theoretical model that describes selective ion transport in electrodialysis systems treating multicomponent (greenhouse) wastewater. The motivation is to reduce freshwater consumption and nutrient losses in greenhouse horticulture while preventing the accumulation of harmful ions such as sodium. Unlike reverse osmosis, which removes both harmful and beneficial ions, electrodialysis offers the potential for selective ion removal.
The research develops a multi-ion transport model that simultaneously accounts for several relevant ions (for example Na^+, K^+, Mg^{2+}, Cl^-, NO_3^-). The model combines channel mass balances with membrane transport described by the Nernst–Planck equation, including diffusion and electromigration. Validation is performed using operational data from a two-stage electrodialysis pilot installation treating horticultural wastewater in Westland. Overall, this research aims to improve understanding of ion selectivity in electrodialysis.

19 Mohammed Qasim - Mechanistic Modeling of Coupled Bio-Electrochemical Processes in Biophotovoltaic Systems

Mohammed Qasim, Luis F.M Rosa, Cristian Picioreanu, Bin Lai

Biophotovoltaic (BPV) systems integrate oxygenic photosynthesis with electrochemical processes, resulting in a tightly connected environment in which biological activity, redox reactions, and aqueous chemistry constantly interact. While these interactions appear to influence system performance, their total impact under dynamic operating conditions is not fully understood, especially across several time periods. To interpret tests and guide system development, it is critical to understand how biological and electrochemical processes interact to shape BPV behavior.
In this study, a time-resolved, zero-dimensional numerical model is constructed to represent coupled bio-electrochemical processes in a batch-operated BPV reactor. The modeling framework incorporates oxygenic photosynthesis, biomass growth, extracellular electron transfer, and anodic redox reactions, while also accounting for dynamically changing aqueous chemistry and gas-liquid mass transfer, in accordance with established bio electrochemical system modeling approaches. Fast acid-base reactions are treated kinetically, allowing system-level variables to develop from first principles rather than being specified.
The model is used to study BPV performance under dynamic working conditions, including as light-dark cycling and electrochemical polarization. According to simulations, electrochemical reactions have a substantial influence on the internal chemical environment on short time scales, while biological development and metabolism

dominate long-term system evolution. These patterns are consistent with previous experimental findings for BPV and comparable bio electrochemical systems. The simulations also demonstrate that transient system responses arise from interactions between electrochemical current production, redox mediator cycling, and aqueous buffering, highlighting dynamics that cannot be described using steady-state or strictly growth coupled descriptions alone. Overall, the model provides a mechanistic platform for investigating process interactions in biophotovoltaic systems as well as interpreting experimental data under dynamic conditions. This work advances the systematic development, comparison, and evaluation of BPV reactors from an electro kinetic standpoint by explicitly coupling biological and electrochemical processes within a unified framework.

20 Richard Dunkel - Enhancing Overlimiting Current Densities in Electrodialysis via Flow Manipulation by Spacers

Richard Dunkel, Michael Garthe, Matthias Wessling

The development of cost-effective electrodialysis (ED) processes operating beyond the limiting current density offers advantages such as lower capital investment and improved energy efficiency. However, such operation is limited by a significant increase in resistance once the limiting current density is exceeded. This study examines whether specifically shaped spacer geometries can mitigate concentration polarization by enhancing local hydrodynamics, thereby enabling more efficient overlimiting current operation. Spacer structures were designed, fabricated using 3D printing, and experimentally evaluated through current–voltage (I–V) measurements. In parallel, three-dimensional computational fluid dynamics (CFD) simulations were carried out to investigate how spacers alter the local flow field and electric current distribution. We hypothesize that spacer geometries that maximize wall-shear stress and maintain lateral velocity homogeneity will delay concentration polarization and raise the overlimiting current in ED. Furthermore, we investigate how the orientation of the ED cell affects the spacer's influence by comparing buoyancy stable and -unstable configurations. In the absence of gravitational convection, cells equipped with advanced spacer designs exhibit longer transition times compared to spacerless configurations, indicating enhanced ion transport toward the membrane.

21 Bryan Enrique Acosta Angulo - Exploring Self-discharge Kinetics on Alkaline Stacks Using Microkinetic Modelling

Bryan Acosta-Angulo, Christodoulos Chatzichristodoulou, Thijs de Groot, John van der Schaaf

A mechanistic mathematical model based on elementary electrochemical steps was developed to describe the self-discharge dynamics of bipolar alkaline electrolyzer stacks. The model incorporates the effective electrode capacitance and the kinetics of surface redox processes to account for reverse currents following a system shutdown. The temporal evolution of cell potentials was obtained by coupling charge balance equations with microkinetic expressions for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). The simulations indicate that the overall discharge time is proportional to the number of cells in the stack, consistent with the larger amount of stored energy. While the electrode capacitance strongly influences the characteristic discharge timescale, the microkinetic description of OER and HER introduces additional nonlinear effects. As the electrode potentials relax toward the stack equilibrium potential, changes in surface coverage and shifts in the rate-limiting elementary steps modify the effective

reaction rates and, consequently, the transient response. Although the identified parameters are system-dependent, the results demonstrate that an accurate representation of elementary reaction mechanisms is essential to capture transient behaviour during dynamic operation of alkaline electrolyzers. However, further incorporation of degradation kinetics is required to elucidate long-term performance losses and to guide strategies for improving the durability of nickel-based electrodes under intermittent operation.

22 Soumyadeep Paul - A stirred-tank flow-electrode reactor for lithium extraction from brines

Soumyadeep Paul, Yousif M. Alkhulaifi, Tomek M. Jaroslawski, Dante Gere, Xuanqi Fang, Ashton M. Aleman, Zhaobang Hou, Wrayzene L. Willoughby, Ryan T. Hannagan, Joseph C. Klewicki, Adam C. Nielander, Thomas F. Jaramillo, Steven A. Hawks, and Juan G. Santiago

Global lithium demand has risen rapidly with widespread lithium-ion battery deployment, and this has intensified interest in selective Li recovery from low-grade brines. These resources often contain <200 ppm Li and high concentrations of competing cations such as Na+, K+, and Ca2+. To date, flow-electrode concepts for direct lithium extraction (DLE) have largely relied on cell architectures that pump slurries through long, thin millimeter-scale channels. These geometries aim to increase surface-to-volume ratio and reduce ionic resistance, but they are difficult to seal, prone to clogging, and difficult to scale. Here, we introduce a new flow electrode DLE architecture that uses a stirred-tank slurry electrode composed of particles of iron phosphate (FePO4) and carbon black within a vigorously stirred tank. Stirring sustains particle motion and causes frequent collisions of particles with a cathode collector and with each other. These collisions facilitate electron transfer to the $FePO_4$ particle phase and drive selective Li intercalation. In lab-scale experiments, the reactor achieves Li/Na intercalation selectivity up to 280 and current densities up to 1 mA cm^{-2}, with low impedance and high intercalation rates despite a small cathode area. We will present the reactor design and an experimental study of this system, including measurements of key performance metrics.

23 Mangut Sunday Jikmyan - Influence of polycation overcompensation on single-salt transport in polyelectrolyte multilayer nanofiltration membranes

Mangut Sunday Jikmyan, Jeffery Wood, Rob Lammertink, Wiebe de Vos

This research investigates the effect of polycation overcompensation in polyelectrolyte multilayer (PEM) nanofiltration membranes on single-salt transport. Using PDADMAC/PSS and PAH/PSS systems as models, a 50 nm thick membrane is simulated, consisting of a negatively charged 6.25 nm top layer and a 43.75 nm bulk layer with varying degrees of polycation overcompensation. Four bulk charge conditions are examined: high, medium, low, and neutral charge, to understand how charge variation affects ion transport across the membrane.
The system is modeled in COMSOL Multiphysics using a one-dimensional Poisson–Nernst–Planck (PNP) framework. A key feature of this study is the inclusion of dielectric exclusion, incorporated through the Freger Born model to correct the activity coefficients. Previous studies often ignored this dielectric term, leading to unrealistically high imposed membrane charge densities (up to 1000 mM) and poor agreement with experimental salt rejections, especially for $MgSO_4$ and NaCl. By accounting for dielectric exclusion, our model achieves realistic rejection values using a reasonable dielectric constant and membrane charge density of 40 and 150 mM, respectively, aligning closely with

experimental data.
The approach highlights the crucial role of dielectric and Donnan exclusion in describing ion transport through PEM nanofiltration membranes. Ongoing work aims to fit the model to experiments to estimate key membrane parameters such as polymer mesh size, dielectric constant, and effective membrane charge density.

24 Valeria M. Günther - Treatment of PFAS Contaminated Landfill Leachate Using Flow-electrode Capacitive Deionization

Valeria M. Günther (a,b), Julius C. Bettermann (a), Christian J. Linnartz (a,b), Matthias Wessling (a,b)

Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants frequently detected in landfill leachate and industrial wastewaters. Their chemical stability, mobility, and resistance to biological degradation make effective treatment challenging. Conventional technologies such as granular activated carbon (GAC) and ion exchange resins are widely applied but often suffer from rapid exhaustion in complex matrices and generate secondary waste streams without enabling controlled concentration. Therefore, alternative treatment strategies that combine selective separation and targeted PFAS management are of increasing interest.
Flow-electrode capacitive deionization (FCDI) is an electro-membrane process that transports ions across ion-exchange membranes into a slurry of activated carbon particles, where they are stored capacitively. This hybrid mechanism may enable PFAS removal either via adsorption onto activated carbon within the flow electrode or via electrically driven transport across anion exchange membranes (AEMs), potentially allowing concentration into a reduced secondary stream. However, the dominant removal pathway and the interaction between PFAS, activated carbon, and ion-exchange membranes under FCDI conditions remain insufficiently understood.
This study systematically investigates PFAS removal in FCDI using perfluorooctanoic acid (PFOA) as a model compound. Adsorption experiments are conducted to evaluate the suitability of the activated carbon employed in the flow electrode. Membrane sorption behavior and transport limitations are analyzed to determine whether AEMs facilitate permeation or act as adsorption sinks. Based on these findings, an adapted FCDI configuration is assessed with respect to its potential to electrically concentrate PFAS into a smaller secondary stream. In addition to model compound experiments, validation tests are performed with real PFAS-contaminated landfill leachate to evaluate matrix effects and practical applicability.

25 Guillermo - Selective metal recovery by an electroleaching process in the FIREFLY project

Guillermo Pozo, Ainhoa Unzurrunzaga, Carmen, del Rio

The EU is the world's top consumer of Platinum Group Metals (PGMs) and is becoming highly dependent on imports, which are essential for its economy. Although Europe uses significant amounts of PGMs in its production, around 84% of its supply comes from third countries. There are considerable amounts of end-of-life products containing PGMs in Europe. These products have vast potential for recycling. However, current industrial recycling technologies, such as smelting or hydrometallurgical processes used by large recycling companies, require high energy consumption and leave a negative carbon footprint that harms both human health and the environment. In this context, TECNALIA is working on the EU-funded project, FIREFLY, which aims to develop a process for the selective recovery of PGMs. The technology relies on electrochemistry and milder

electrolytes, which avoid several unit operations and significantly reduce chemical use, improving economy compared to the SoA technologies and reducing GHG emissions. The process uses a combination of organic solvents, including deep eutectic solvents (DES) and mild aqueous NaCl solutions (e.g., 0.5 M), to selectively dissolve metals from solid materials. The polarization of the electrodes will promote the production of oxidizing agents at the anode, such as hydroxyl radicals and hydrogen peroxide (hence avoiding their external addition), releasing the metals from the solid residue. Simultaneous electrodeposition of metals may occur at the cathode, depending on the physicochemical properties of the solid input residues and the operational conditions employed.

26 Peter Burger - Electrochemical recovery of Li-ions from industrial process water

Peter Rolf Burger, Saïd Mondahchouo, Stefanie Arnold, Moritz Petzold, Sabine Flamme, and Volker Presser

The rapid growth of the electric vehicle market has created an urgent need for environmentally friendly lithium-ion battery recycling. Current industrial methods often rely on high-heat smelting or hazardous acid-leaching, both of which produce significant carbon footprints and toxic waste. Our research presents a sustainable, closed-loop lithium recovery workflow that replaces traditional, hazardous hydrometallurgical methods with an integrated aqueous mechanical and electrochemical approach. The process begins with the shredding of spent lithium-ion batteries directly in aqueous media. The resulting process water solution is then used for the electrochemical extraction and recovery of lithium ions utilizing a lithium iron phosphate (LFP) as the working electrode. By leveraging the ion-selective intercalation chemistry of the LFP olivine lattice, we achieve a high-purity lithium solution from this process water solution through a two-step potential-swing protocol consisting of selective capture (intercalation) and controlled release (deintercalation). Electrochemical data confirms high desalination capacity and stable performance over 100 cycles with low energy consumption. This approach offers a safe, low-energy blueprint for the production of high-purity lithium while cutting the chemical footprint of battery production.

27 Yassine Seffar - Selective lithium extraction from aqueous solution by capacitive deionization

Yassine Seffar, Peter Burger, Mouad Dahbi, Volker Presser,

Advanced carbon electrodes are needed to improve the performance of capacitive deionization (CDI) in complex saline waters. In this work, nitrogen–sulfur co-doped activated carbon (N,S-AC) and boron-doped activated carbon (B-AC) electrodes were investigated for lithium-ion selectivity and ion removal in brackish water containing Li^+, Na^+, K^+, Ca^{2+}, and Mg^{2+}. Heteroatom doping enhanced charge distribution, wettability, and ion transport within the electrodes. The N,S-AC electrode showed strong lithium selectivity, while B-AC exhibited higher adsorption capacity. Importantly, B-AC combined high desalination performance with improved lithium selectivity even in the presence of competing Na^+, Mg^{2+}, and Ca^{2+} ions. These findings reveal the complementary roles of N,S co-doping and boron doping, and demonstrate the potential of heteroatom-engineered carbon materials for selective ion removal and lithium recovery in CDI applications.

28 Hanieh Geranikolahlooei - Selective ion removal through process parameters tuning

Hanieh Geranikolahlooei, Sara Vallejo Castanoa, Slawomir Porada, Louis CPM de Smet

Selective ion separation plays an important role in sustainable water treatment and resource recovery, especially when it comes to the separation of similarly sized monovalent ions, such as sodium (Na+) and potassium (K+), because of similar chemical and physical properties.

Capacitive deionization (CDI) is a promising method because of its energy efficiency and low-voltage operation. Using Prussian Blue Analogue (PBA) electrodes like Nikel Hexacyanoferrate (NiHCF) enables selective ion removal through redox-driven intercalation within a crystalline lattice. However, reaching the theoretical selectivity of these materials in practical systems remains challenging. Selectivity may be reduced during operation due to ion depletion, overpotentials at high currents, incomplete equilibrium during cycles, and short operation times.

This study investigates how tuning operational parameters can increase the K^+ over Na^+ selectivity in CDI using NiHCF electrodes. Experimental results show that operating at low current densities and within an intermediate state-of-charge range helps reduce non-selective intercalation. Additionally, adding rest periods between charge/discharge cycles allows the system to reach closer to electrochemical equilibrium, which significantly avoids sodium intercalation while maintaining high potassium selectivity.

29 Sara Vallejo - Efficiency and energy consumption analysis of bipolar membrane electrodialysis for electrochemical CO2 capture

Sara Vallejo-Castaño, Giordana Bianchi, Qingdian Shu, Elise Mathiasin, Michel Saakes, Philipp Kuntke, Hubertus V. M. Hamelers

Bipolar membrane electrodialysis (BMED) is an electricity-driven technology that can capture and purify CO2, but its efficiency remains poorly understood. This work quantified coulombic efficiency losses in BMED for carbon capture using a fully saturated (1 M KHCO3) and a partially saturated KOH solvent. Fully saturated solutions required 50% less energy consumption than partially saturated solutions for CO2 purification and solvent regeneration. The minimum specific energy consumption was 161.2 kJ per mol CO2 (3.65 GJ per ton CO2) at 100 A/m2 and was limited by parasitic potassium transport across the bipolar membrane, resulting in low CO2 desorption efficiency (<60%) at low current density. Additionally, incomplete CO2 desorption represented up to 10% of efficiency losses in most of the conditions tested. BMED displayed 100% CO2 desorption efficiency (mol CO2 per mol e−) and a specific energy consumption of 290.61 kJ per mol CO2 (6.60 GJ per ton CO2) at industrially relevant current densities (1000 A/m2). This work presents a robust analytical framework to identify coulombic efficiency losses and identifies the cause for low CO2 desorption efficiency at a wide range of current densities and operational conditions, providing unique insights into the transport mechanisms in BMED and unlocking new pathways to maximise technology performance.

30 Abhirup Chaudhuri - Surface Charge Heterogeneity Driven Electrokinetics with Ion-Specific Slip Effects in Graphene Nanochannels

Abhirup Chaudhuri, Chirodeep Bakli, Suman Chakraborty

The growing relevance of nanofluidic systems for electrokinetic energy conversion has necessitated a deeper understanding of the interfacial phenomena governing nanoscale transport. In such systems, the electrokinetic response arises from a delicate coupling between the electrical double layer (EDL) structure and interfacial hydrodynamics. Consequently, the surface charge of the confining walls plays a major role in dictating the electrokinetic effect. Moreover, interfacial fluid slippage can significantly amplify electrokinetic behaviour by remobilising otherwise immobile ions within the Stern layer. However, slip and surface charge are inherently coupled, necessitating the identification of an optimal surface charge distribution. Furthermore, the ionic species present in the electrolyte can themselves modulate the effective interfacial charge distribution through ion-specific adsorption and correlations, thereby altering the charge–slip coupling. While prior studies have primarily focused on uniformly charged surfaces, realistic interfaces often exhibit spatial charge heterogeneity, whose implications for electrokinetic transport remain inadequately explored.

In this work, we employ molecular dynamics (MD) simulations using 1 M aqueous solutions of different electrolytes confined within homogeneously and heterogeneously charged graphene nanochannels to investigate the ion-specific effects of surface charge distribution on interfacial slippage. The surface charge is varied from 0 to −0.1 C/m² to optimize the slip–charge-dependent electrokinetic response in graphene nanochannels. A Poiseuille flow is simulated by applying an external force on the liquid molecules along the axial direction of the channel. Subsequently, the Helmholtz–Smoluchowski equation is used to estimate the zeta potential, which quantifies the electrokinetic response. The slip length is determined by enforcing the continuity of tangential stress at the liquid–solid interface along with the Navier slip condition.

While both homogeneously and heterogeneously charged surfaces exhibit a reduction in fluid slippage with increasing surface charge, we demonstrate that the nature of charge distribution fundamentally alters interfacial transport. In contrast to uniformly charged surfaces, heterogeneous charge distributions promote localised counterion accumulation and site-specific adsorption, thereby enhancing interfacial friction and suppressing the slip length. Furthermore, the rate of slip reduction is strongly ion-dependent, with multivalent counterions exhibiting stronger electrostatic correlations and reduced hydration mobility. This results in enhanced ion–surface binding and greater disruption of interfacial water structure compared to monovalent counterions. Consequently, significant modifications in water orientation, hydration layering, and ion–water coupling arise near the interface, collectively influencing both EDL structure and hydrodynamic slip. As a result, the electrokinetic response exhibits a nontrivial dependence on both surface charge distribution and the electrolyte type. While homogeneous surfaces facilitate slip-enhanced electrokinetic amplification, heterogeneous surfaces diminish this enhancement due to frictional penalties associated with ion localization. These findings reveal that optimal electrokinetic performance requires coordinated tuning of surface charge architecture and electrolyte composition, rather than surface charge magnitude alone. Overall, this study provides molecular-level insights into the coupled roles of ion-specific charge–slip interactions in nanoconfined systems, offering design principles for improved electrokinetic energy conversion and nanoscale transport control.

31 Alessandro Gavazzi - Predicting the effect of operational conditions on local hydrogen concentration and pH within 3D porous cathodes

Alessandro Gavazzi, Jos Steller, Jouke Dykstra, Sanne de Smit

Microbial electrosynthesis (MES) is a promising biotechnology that converts CO_2 into valuable organic compounds, supporting the decarbonization of the chemical industry. Electroactive acetogenic bacteria grow on the cathode surface and use the electrochemically generated H_2 in the bioconversion, making local H_2 availability critical for microbial activity. However, MES scale-up remains constrained by low production rates and limited energy conversion efficiency. Porous electrodes have proven effective in this context: their structure provides high specific surface area, supports dense biofilm formation and enhances mass transport. However, spatial heterogeneities in H_2 concentration and pH develop within porous cathodes, impacting microbial activity across different electrode zones. There is currently limited understanding of local chemical environments within porous cathodes and of how reactor design and operational conditions shape them.

A two-dimensional mathematical model was developed to predict how catholyte recirculation design and operating conditions influence dissolved H_2 and pH distributions within a porous graphite felt cathode under abiotic conditions. Predictions were validated against in-situ microsensor measurements under three catholyte recirculation designs.

The model captured H_2 distribution trends across all recirculation designs. H_2 concentration decreased from the membrane toward the current collector, with recirculation hydrodynamics influencing H_2 profiles across the cathode depth. Among the operational parameters tested, flow rate and current density had the greatest impact on local H_2. Reducing flow rate by 20% increased local H_2 by up to 16%, while a 20% increase in current density raised membrane-side H_2 by 25%, intensifying concentration gradients along the cathode depth. pH prediction remained limited, likely due to inaccuracies in microsensor measurements.

These findings provide quantitative guidelines for optimizing catholyte recirculation design and operating conditions in MES reactors, supporting more rational design strategies for porous cathodes towards scaled-up systems.

32 Subradip Debnath - Electrokinetic control of interfacial thermal transport in nanoconfined electrolytes

Subradip Debnath, Chirodeep Bakli and Suman Chakraborty

Interfacial thermal resistance, commonly expressed as the effective Kapitza length (L_(k-eff)), fundamentally constrains heat transport at the nanoscale and sets performance limits for emerging thermal management and energy-conversion technologies. Although surface chemistry and temperature effects have been extensively examined for idealised solid–liquid interfaces, how ion identity, hydration structure, and concentration interact with graphene–water interfaces to regulate electroosmotic flow and interfacial thermal resistance has not yet been systematically resolved. This lack of understanding linking interfacial heat transfer with electrical double-layer (EDL) physics obscures the molecular origins of interfacial resistance and limits the rational design.
Here, we employ non-equilibrium molecular dynamics simulations to systematically investigate the coupled influence of wetting strength, electrolyte concentration, and temperature in graphene-confined electrolyte systems. By considering a range of ions with distinct sizes and hydration characteristics, along with temperatures spanning 300–370 K, we elucidate the molecular origins of interfacial thermal resistance and electrokinetic response. Temperature profiles are used to extract Kapitza resistance and the corresponding effective Kapitza length (L_(k-eff)), while ionic and water density

distributions are used to characterise the interfacial structuring length scale. Surface potential energy[1] derived from atomistic simulations is used as an indirect descriptor of the interfacial electrostatic field strength. To bridge electrostatic and thermal transport, we introduce the Debye length (λ_D) as an electrostatic analogue of L_(k-eff). The two length scales are found to be interrelated: systems exhibiting shorter λ_D, indicative of stronger charge screening at higher ion concentrations, display enhanced interfacial heat flux and reduced L_(k-eff). Furthermore, ion identity strongly modulates both electroosmotic flow and interfacial heat transfer. L_(k-eff) decreases with ion size and hydration strength, reflecting the role of interfacial water structuring and ion–surface interactions. With increasing temperature, the magnitude of the electroosmotic mobility (v_e) decreases, indicating a weakening of the interfacial electrostatic environment; this effect is accompanied by a general increase in L_(k-eff), consistent with the disruption of hydrogen-bond networks at elevated temperatures. Importantly, a direct relationship between interfacial thermal resistance and the electrokinetic transport coefficient is established, indicating that conditions favouring shorter λ_D, compact double layers, and strong electroosmotic flow also promote more efficient interfacial heat transfer. Overall, this study provides a unified molecular-level understanding of coupled thermo–electrokinetic transport in graphene nanoconfinement and introduces a physically consistent mapping between thermal and electrostatic interfacial phenomena. These insights offer actionable design principles for optimising graphene-based nanofluidic systems in applications such as blue energy harvesting, thermal management, and electrochemical energy conversion.

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33 José Agustín Epstein - Permeability modulation via poroelastic–osmotic coupling in a charged hydrogel layer

José Agustín Epstein, Andrij Pich, Matthias Wessling

Transport in fouled nanofiltration membranes can be strongly influenced by cake-enhanced concentration polarization, whereby ion accumulation within the fouling layer elevates the effective osmotic pressure and governs permeation. In charged polymeric foulants, this effect is further modulated by interactions between counter-ions and the soft porous matrix. In this work, we experimentally show that periodic pressure waveforms induce asymmetric permeation dynamics arising from swelling and compaction of the fouling layer. Using a microfluidic nanofiltration platform, we probe permeability under periodic pressure waveforms, revealing nonlinear and hysteretic permeate flux responses associated with these dynamics and their characteristic relaxation times.

The interplay between poroelastic deformation (of the foulant layer) and concentration polarization leads to a time-dependent permeability that depends on waveform properties. During pressure release, osmotic backflow can emerge due to ion accumulation within the fouling layer. Under periodic pressure waveforms, certain shapes enhance net permeation relative to steady conditions, while others reduce performance. These results indicate that poroelastic–osmotic coupling governs the observed transient permeability.

34 Maarten Biesheuvel - The second law of Friedrich Kohlrausch (1885)

Friedrich Kohlrausch (1840-1910) is known for his first and second laws on ionic conductivity. He formulated his second law in 1885 which deals with the dependence of specific (or, molar) conductivity on salt concentration. Between 1885 and 1898 he wrote several papers showing that conductivity data are very well described by a dependence on the cube root of salt concentration. A theoretical model by Hertz in 1912 is in perfect agreement with the second law of Kohlrausch. An intriguing deviation was found by Kohlrausch for concentrations below 0.1 mM, and is also predicted by the theory of Hertz.

35 Larysa Lysenko - Effect of electric field on behavior of uncharged impurities in concentrated clay dispersions

Fine disperse clay systems are objects of treatment within the field of environmental protection. Primarily, this concerns the removal of toxicants of various natures from them. However, specific surface and bulk characteristics of this systems, such as large specific surface area, heterogeneous surface charge, and the narrowness and tortuosity of the pore space, require a thorough approach to the choice of separation method. Electrokinetic treatment demonstrates an optimal compromise between the degree of decontamination and energy consumption in comparison with other methods.

The main transport flows that take place in dispersions when using an electric field are electroosmosis, electromigration, and diffusion. When selecting the parameters for the separation process, it is necessary to consider that transport flows are influenced not only by the properties of the dispersion and the toxicant but also by the changes occurring in the system as a result of electrode reactions. The generation of hydroxyl and hydrogen ions at the cathode and anode leads to the emergence of local pH inhomogeneity in the dispersion medium, which, in turn, causes changes in the surface charge, electroosmotic velocity, solubility of toxicants, etc. Additionally, a redistribution of the electric field occurs within the system, and polarization processes are intensified. Consequently, the pH value of the dispersion medium is one of the main parameters that must be regulated during treatment. One of the ecologically acceptable ways to accelerate and enhance electrokinetic remediation is the electrohydrodynamic pH control by selecting the pumping rate of neutral electrolytes in electrode chambers [1].

In the removal of uncharged organic pollutants from dispersions, treatment efficiency is determined by the velocity and stability of the electroosmotic flow, the possibility of desorption and solubility of the organic compound in the dispersion medium, as well as diffusion processes. In the case of hydrophobic substances, surfactants must be used to convert them into a water-soluble state [2].

Taking into account the main factors influencing the electroosmotic transport of uncharged hydrophobic organic pollutants in concentrated clay dispersions, a comprehensive theoretical and experimental study on their electrokinetic purification was conducted. A scientific framework has been developed that combines changes in the pH of the dispersion medium, the velocities of electroosmotic and diffusive transport of toxicants and surfactants, as well as the hydrodynamic flows arising in the narrow pore space of fine disperse systems. To minimize the impact on the surface charge, the use of non-ionic surfactants is optimal. Research on the concentration of surfactants as they pass through the dispersion showed a significant decrease, which is caused by both interaction with dispersed particles and the steric factor. Accordingly, for the effective removal of toxicants, initial concentration levels were determined that ensure the critical micelle concentration of the surfactants used is exceeded at the system's outlet. The main

process parameters were established under which stable electroosmotic removal of uncharged hydrophobic organic compounds from concentrated clay dispersions occurs.

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