

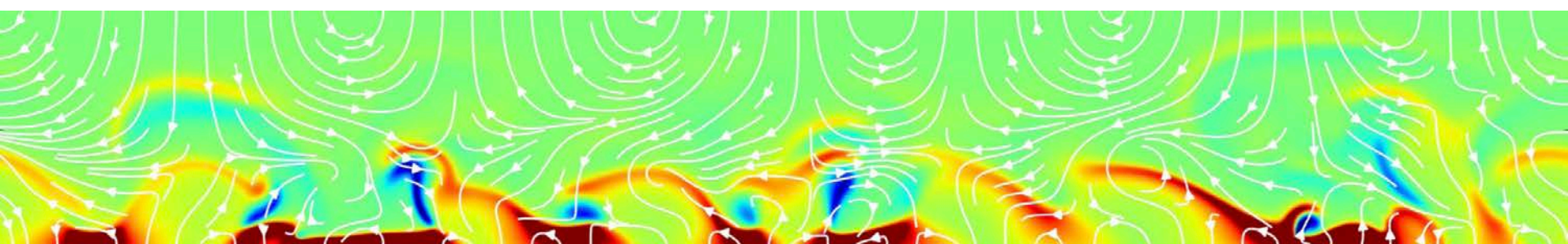
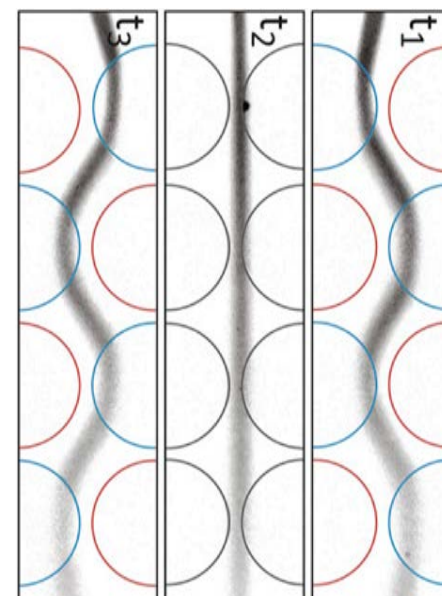
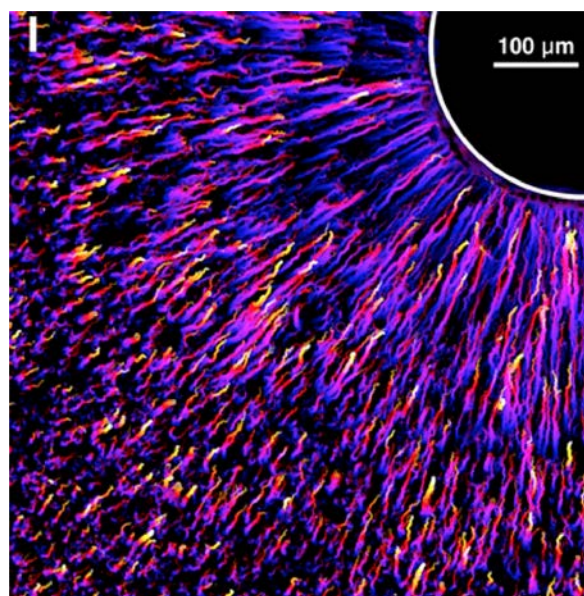
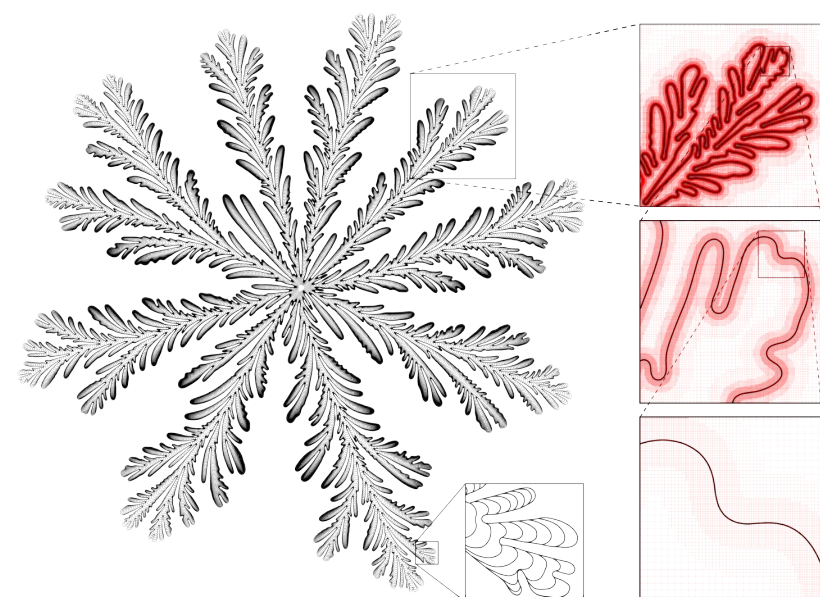
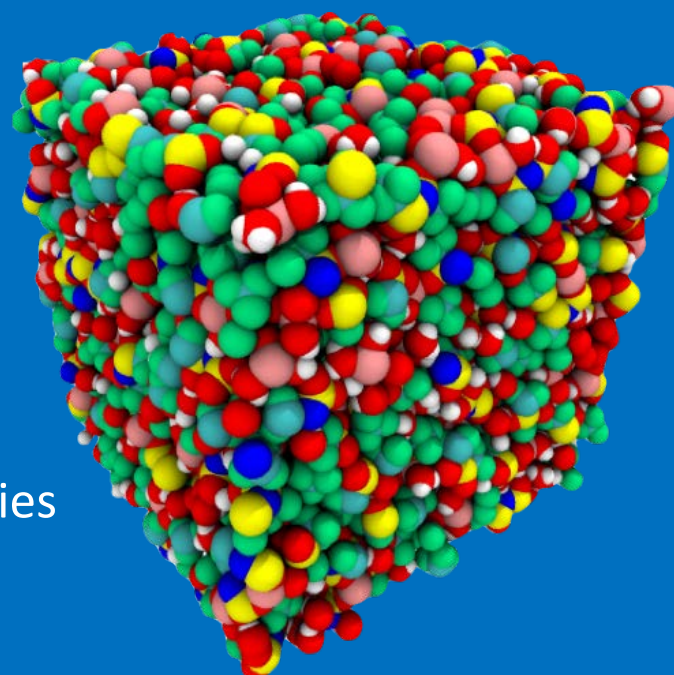
13th International Symposium on Electrokinetics

Cambridge, MA, United States

June 12-14, 2019

elkin2019.mit.edu

- Micro/nanofluidics
- Electrophoresis, diffusiophoresis, and colloids
- Electrohydrodynamics and electrokinetic instabilities
- Structure and dynamics of electrical double layers
- Biological electrokinetics and electro-physiology
- Flow batteries and electrokinetic energy conversion
- Electrokinetics for the oil and gas industry
- Mathematical modeling and simulation



MIT Campus Map

Welcome to MIT

All MIT buildings are designated by numbers. Under this numbering system, a single room number serves to completely identify any location on the campus. In a typical room number, such as 7-121, the figure(s) preceding the hyphen gives the building number, the first number following the hyphen, the floor, and the last two numbers, the room.

Please refer to the building index on the reverse side of this map, if the room number is unknown.

Use the online campus map:
<http://whereis.mit.edu/>

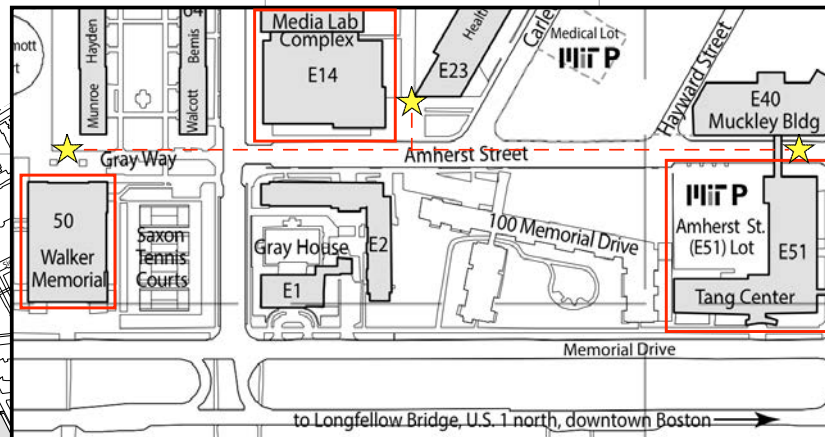
Find your way around campus with your phone: <http://m.mit.edu>

Parking

= public parking (pay lots)

= MIT permit parking

Building Entrance



Media Lab (E14)
- Banquet

Note: Take the elevator to the 6th floor

Walker Memorial (50)
- Poster Session
- Lunch

Note: Poster session and lunch are held in the main hall

Tang Center (E51)
- Registration
- Oral Sessions

Note: All talks are held in the Wong Auditorium (E51-115)

Massachusetts Institute of Technology

revised September 2018

MIT campus map index (Building number follows name)

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Visitor information

As parking is limited and regulations are aggressively enforced, visitors are strongly encouraged to use public transportation.

By public transportation, MBTA ("The T")

A parking garage at Alewife Station (Routes 2 and 16 at the Cambridge/Belmont/Arlington line) allows access to the Red Line subway. Take the Red Line from Alewife Station in Cambridge or from Park Street Station in Boston to Kendall/MIT Station or to the Central Square Station, both of which are within walking distance of MIT. There is regular MBTA bus (#1) service along Massachusetts Avenue from MIT to Boston and Harvard Square.

From Logan Airport by MBTA

Taxi fare is about \$20–\$30. To travel by subway, at Logan Airport take the airport shuttle bus that runs to the Blue Line Subway Station. Take the Blue Line to the Government Center Station and go upstairs to board the Green Line Trolley to Park Street. At Park Street Station go downstairs to board the Red Line Subway going outbound towards Alewife and exit at Kendall/MIT or Central Square Station.

By car from Logan Airport

Leaving the airport follow the signs to the Summer Tunnel. Entering the tunnel keep in the right lane for Storrow Drive North. Continue in the right lane following the Storrow Drive West signs. Exiting the tunnel you will see the Massachusetts Eye and Ear Infirmary on your left and the Charles River on your right. Keep to the right and continue to follow the Storrow Drive West signs. After passing under the Arthur Fiedler pedestrian walk bridge, change to the left lane and take exit for Massachusetts Avenue/Cambridge (2AN). Bear right and cross the Harvard Bridge. MIT's main entrance at 77 Massachusetts Avenue will be on your right, at the third set of traffic lights.

By car from Route I-93 or Southeast Expressway

Take exit 26. Keeping in the right lane, follow the Storrow Drive West signs. After passing under the Arthur Fiedler pedestrian walk bridge, change to the left lane and take exit for Massachusetts Avenue/Cambridge (2AN). Bear right and cross the Harvard Bridge. MIT's main entrance at 77 Massachusetts Avenue will be on your right, at the third set of traffic lights.

By car from Route I-90

Take the Cambridge/Allston Exit (18) on the left off of the Massachusetts Turnpike (Interstate 90). Bear right at the end of the ramp and go through two sets of traffic lights. Follow the signs to Cambridge. Cross the River Street Bridge and continue straight ahead for about one mile to Central Square. Turn right onto Massachusetts Avenue. MIT's main entrance, 77 Massachusetts Avenue, is about one-half mile down on the left.

By car from Route I-95 low the I-93 directions to MIT as given. From the south take I-90 off of I-95 and follow the I-90 directions to MIT as given.

Call a taxi

Yellow Cab: 617-492-0500

Parking

Ⓟ = public parking (pay lots) MIT P = MIT permit parking

Campus telephones

MIT house telephones are located in many of the campus lobbies including the Student Center (map section D). To reach an office extension from a house telephone dial the last 5 digits (i.e. 3-4795) of the number. To contact a person, department, or residence at MIT, dial 0 from a house phone or 617-253-1000.

Campus tours

Tours of campus: 11:00 am and 3:00 pm weekdays except holidays. Tours leave from 77 Massachusetts Avenue, Lobby 7 (map section D). Admissions Office undergraduate information sessions: 10:00 am and 2:00 pm (preceding tour) from mid-March through mid-December except holidays. Confirm at <http://web.mit.edu/admissions>.

Dining on campus

Snacks and meals are available in the Student Center (map section D) and in the Stata Center (map section E). There are restaurants and small eating places in the Kendall Square area of the campus and in the local hotels adjacent to the campus.

The MIT Press

One of the country's largest university presses, the MIT Press publishes books and journals circulated throughout the world. Its titles include professional, reference, and scholarly books; graduate and undergraduate texts and books for general audiences. The MIT Press Bookstore is located at 301 Massachusetts Ave (N50, map section C2).

MIT events and exhibits

The MIT Events Calendar is available online at <http://calendar.mit.edu>.

A map giving locations of the public art in MIT's Permanent Collection, overseen by the List Visual Arts Center, may be found at <http://listart.mit.edu/public-art-map>.

The following 24-hour numbers are available for recorded information on current arts events:

- Concerts 617-253-9800
- List Visual Arts Center 617-253-4680
- MIT Museum 617-253-4444
- Theater Arts 617-253-4720

Student center facilities

W20 - 84 Massachusetts Avenue (map section D3)

- Bank, 1st floor
- Caterina, 2nd floor
- Campus Police/event registration detail, basement
- Cleaners, basement
- Conor Moran Lounge, 5th floor
- MIT Copytech, 1st floor
- Food Market/convenience store, 1st floor
- Game Room, 1st floor
- Hair salons, basement
- Manager, Campus Activities Complex, 5th floor
- Optical Store, basement
- Police, Detail Office, W20-020B
- Post Office (U.S.), basement
- Restaurants, 1st and 2nd floors
- Stratton Lounge, Catherine N., 2nd and 3rd floors
- Tech Coop, 1st floor (no textbooks)
- Wiesner Student Art Gallery, 2nd floor

For more information

- Massachusetts Institute of Technology
- Information Center
- Room 7-121
- Telephone 617-253-4795
- <http://web.mit.edu>
- 77 Massachusetts Avenue
- Cambridge, MA 02139-4307



13th International Symposium on Electrokinetics,

Cambridge, MA, United States

June 12 – 14, 2019



Wednesday, June 12		Thursday, June 13		Friday, June 14	
8:00	Registration <i>Tang Center Entrance (E51)</i>	8:00	Registration <i>Tang Center Entrance (E51)</i>	8:00	Registration <i>Tang Center Entrance (E51)</i>
9:00	Conference Opening <i>Wong Auditorium (E51-115)</i>	9:00	Keynote Lecture (K2) <i>Wong Auditorium (E51-115)</i>	9:00 Bio-electrokinetics (C5) <i>Wong Auditorium (E51-115)</i>	
9:15	Electrokinetics in Oil & Gas Industry (S1) <i>Wong Auditorium (E51-115)</i>	9:45	Ionic Liquids (S2) <i>Wong Auditorium (E51-115)</i>		
10:45	Coffee Break <i>Ting Foyer (E51)</i> 	10:45	Coffee Break <i>Ting Foyer (E51)</i> 	10:45	Coffee Break <i>Ting Foyer (E51)</i> 
11:00	Keynote Lecture (K1) <i>Wong Auditorium (E51-115)</i>	11:00	Keynote Lecture (K3) <i>Wong Auditorium (E51-115)</i>	11:00	Keynote Lecture (K4) <i>Wong Auditorium (E51-115)</i>
11:45	Poster Soundbites (PS1) <i>Wong Auditorium (E51-115)</i>	11:45	Poster Soundbites (PS2) <i>Wong Auditorium (E51-115)</i>	11:45	Poster Soundbites (PS3) <i>Wong Auditorium (E51-115)</i>
12:30	Poster & Lunch (P1) <i>Walker Memorial (50, Main Hall)</i>	12:30	Poster & Lunch (P2) <i>Walker Memorial (50, Main Hall)</i>	12:30	Poster & Lunch (P3) <i>Walker Memorial (50, Main Hall)</i>
14:00	EK & EHD Instabilities (C1) <i>Wong Auditorium (E51-115)</i>	14:00	Microfluidics (C3) <i>Wong Auditorium (E51-115)</i>	14:00	Physics of Membranes (S3) <i>Wong Auditorium (E51-115)</i>
15:45	Coffee Break <i>Ting Foyer (E51)</i> 	15:45	Coffee Break <i>Ting Foyer (E51)</i> 	15:45	Coffee Break <i>Ting Foyer (E51)</i> 
16:00	Mathematical Modeling (C2) <i>Wong Auditorium (E51-115)</i>	16:00	Colloids & Interfaces (C4) <i>Wong Auditorium (E51-115)</i>	16:00	Physics of Membranes (S4) <i>Wong Auditorium (E51-115)</i>

Wednesday, 12 June

8:00	Registration <i>Tang Center Entrance (E51)</i>
9:00	Conference Opening <i>Wong Auditorium (E51-115)</i>
9:15	Electrokinetics in Oil & Gas Industry (S1) <i>Wong Auditorium (E51-115)</i> Chaired by: Dr. Mohammad Mirzadeh
9:15	Electrokinetic Phenomena in Oil Recovery and Production: From Theory to applications » <u>Dr. Amr Abdel-Fattah</u>
9:45	Sculpting Diffusiophoretic Migration with Reactive Solutes » <u>Dr. Xiaoyu Tang</u> , Dr. Nan Shi, Mr. Anirudha Banerjee, Dr. Amr Abdel-Fattah, Dr. Afnan Mashat, Prof. Todd Squires
10:00	Zeta potential of the mineral-brine interface in natural, intact carbonates: implications for improved oil recovery by controlled salinity waterflooding. » <u>Prof. Matthew Jackson</u> , Mr. Harry Collini
10:15	Induced Polarization Due To Dispersed Electronic Conductors in Brine-Filled Porous Media » Dr. Lang Feng, Dr. Qiuzi Li, Dr. Stephen Cameron, Dr. Harry Deckman, <u>Dr. Deniz Ertas</u>
10:30	Electrochemical transformation of crude oils in electrokinetic recovery » <u>Prof. Ehsan Ghazanfari</u> , Prof. Sibel Pamukcu, Prof. Mesut Pervizpour
10:45	Coffee Break <i>Ting Foyer (E51)</i>

11:00	Keynote Lecture (K1) <i>Wong Auditorium (E51-115)</i> Chaired by: Prof. Martin Bazant
11:00	Electroconvection in membrane systems: experiment, modelling and applications to electrodialysis » <u>Prof. Victor Nikonenko</u>
11:45	Poster Soundbites (PS1) <i>Wong Auditorium (E51-115)</i>
11:45	Modelling of field-induced orientation and impedance in suspensions of conductive and insulating ellipsoids: Is the orientation determined by the principle of maximum entropy production? » <u>Prof. Jan Gimsa</u>
11:50	Electrokinetic instability at an extremely non-equilibrium electrophoresis of ion-selective microparticle » <u>Ms. Elizaveta Frants</u> , Dr. Georgy Ganchenko, Dr. Vladimir Shelistov, Dr. Sakir Amiroudine, Dr. Evgeny Demekhin
11:55	Role of Stefan-Maxwell fluxes in the dynamics of concentrated electrolytes » <u>Ms. Bhavya Balu</u> , Prof. Aditya Khair
12:00	Induced Charge Electroosmotic Flow Including Finite Ion Size Effects » <u>Dr. Jürgen Fuhrmann</u> , Dr. Alexander Linke, Dr. Christian Merdon, Dr. Rüdiger Müller
12:05	Theoretical and Experimental Investigations of Electroosmotic Flow Beyond Debye-Hückel Regime » Mr. Anil Koklu, Dr. Alper Tunga Celebi, <u>Prof. Barbaros Cetin</u> , Prof. Ali Beskok
12:10	Autonomous NanoSurfactant for Enhanced Oil Recovery Applications » Dr. Nan Shi, <u>Dr. Afnan Mashat</u> , Dr. Amr Abdel-Fattah

Continued from **Wednesday, 12 June**

12:15 **Automated In-Situ Wettability Characterization on Reservoir-on-a-chip Using Deep Learning**

» [Dr. wonjin yun](#), Dr. Sehoon Chang, Prof. Anthony R. Kovalick

12:20 **Insights into the Electrokinetic Effects on Oil Recovery at the Pore-Scale in Carbonate Rocks**

» [Dr. Moataz Abu-Al-Saud](#)

12:30 **Poster & Lunch (P1)**

Walker Memorial (50, Main Hall)

1 **Modelling of field-induced orientation and impedance in suspensions of conductive and insulating ellipsoids: Is the orientation determined by the principle of maximum entropy production?**

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8 **Insights into the Electrokinetic Effects on Oil Recovery at the Pore-Scale in Carbonate Rocks**

» [Dr. Moataz Abu-Al-Saud](#)

9 **Temperature-gradient-induced electrokinetic transport of electrolyte solutions in charged capillaries**

» [Mr. Wenyao Zhang](#), Prof. Qiuwang Wang, Prof. Min Zeng, Prof. Cunlu Zhao

10 **2D Patterned Ion-Exchange Membranes Induce Electroconvection**

» [Mr. Felix Stockmeier](#), Mr. Florian Roghman, Ms. Elizaveta Evdochenko, Mr. Sven Schneider, Mr. Amel Smailji, Dr. Rahul Tiwari, Ms. Annabel Mikosch, Dr. Elif Karatay, Prof. Alexander Kühne, Prof. Andreas Walther, Prof. Ali Mani, Prof. Matthias Wessling

11 **Dielectrophoretic-driven deformations of a lubricated elastic sheet**

» [Mr. Israel Gabay](#), Ms. Vesna Bacheva, Prof. Amir D. Gat, Prof. Moran Bercovici

12 **Elastic instability in soft microfluidic configurations driven by non-uniform electro-osmotic flow**

» [Mr. Evgeniy Boyko](#), Prof. Moran Bercovici, Prof. Amir D. Gat

13 **The effect of electroconvective instability on the transient response of a microchannel-nanochannel interface device**

» [Mrs. Neta Zalmanovich](#), Dr. Ramadan Abu-Rjal, Prof. Gilad Yossifon

Continued from **Wednesday, 12 June**

- # 14 Electroconvection at an anion-exchange membrane in NaH₂PO₄ and NaCl solutions**
» Prof. Natalia Pismenskaya, Prof. Victor Nikonenko, Dr. Semyon Mareev, Mrs. Olesia Rybalkina, Ms. Kseniya Tsygurina
- # 15 Electroconvective Instability on High Water-permeable Ion-selective Membrane**
» Mr. Dokeun Lee, Prof. Hyomin Lee, Prof. Sung Jae Kim
- # 16 Electrokinetic Induced Wettability Alteration in Carbonates**
» Mr. Amani Alghamdi
- # 17 Zeta potential of the mineral-brine interface in natural, intact sandstones with oilfield applications**
» Mr. Harry Collini, Prof. Matthew Jackson
- # 18 Understanding Calcium-Mediated Adhesion of Nanomaterials in Reservoir Fluids: Insights from Molecular Dynamics Simulations**
» Dr. Hsieh Chen, Dr. Shannon Eichmann, Prof. Nancy Burnham
- # 19 Understanding the Impact of Hybrid Nano Acid Fluid (HNAF) Pulsed with Electrokinetic (EK) stimulation in Tight Carbonate Reservoirs**
» Dr. Mohamed Haroun, Prof. George Chilingar
- # 20 Relationship Integrating Zeta Potential and Displacement Efficiency: A Novel Approach Towards Smart Waterflooding Mechanism**
» Dr. Mohamed Haroun, Prof. George Chilingar
- # 21 Hydrodynamic and electrokinetic transport of liquid and microparticles in porous materials**
» Dr. Larysa Lysenko, Prof. Nataliya Mishchuk, Dr. Nataliya Barinova
- # 22 Active Control of Viscous Fingering Using Electric Fields**
» Dr. Tao Gao, Dr. Mohammad Mirzadeh, Prof. Martin Bazant

- # 23 Effect of pulsed electric field on electroconvection according to the relaxation time of convection**
» Mr. Soonhyun Kwon, Prof. Hyomin Lee, Prof. Sung Jae Kim
- # 24 Targeting colloidal particle delivery into dead-end pores using solute gradients generated in situ**
» Dr. Huanshu Tan, Mr. Anirudha Banerjee, Mr. Parth Shah, Mr. David Taylor, Dr. Afnan Mashat, Dr. Amr Abdel-Fattah, Prof. Todd Squires
- # 25 Numerical analysis of three-dimensional electrohydrodynamic instability in crossflow**
» Mr. Yifei Guan, Prof. Igor Novosselov
- # 26 Electrokinetic control of miscible flow instabilities in porous media**
» Dr. Amin Amooie, Dr. Mohammad Mirzadeh, Prof. Martin Bazant
- # 27 Electro-osmosis in Liquid Foam**
» Dr. Baptiste Blanc, Dr. Oriane Bonhomme, Prof. Laurent Joly, Prof. Christophe Ybert, Prof. Anne-Laure Biance
- # 28 Ionic current magnetic fields in charged 3D nanoslits**
» Prof. Abraham Mansouri

14:00 EK & EHD Instabilities (C1)
Wong Auditorium (E51-115)
Chaired by: Prof. Ali Mani

14:00 Equilibrium Electro-convective Instability in Electrodeposition with Butler-Volmer Kinetics
» Prof. Isaak Rubinstein, Prof. Boris Zaltzman

14:30 Orientation effects in hydrodynamic instability in concentration polarization
» Dr. Pramoda Kumar, Prof. Isaak Rubinstein, Prof. Boris Zaltzman

Continued from **Wednesday, 12 June**

- 14:45 **Ion concentration polarization in micro/nanofluidic platforms**
» [Prof. Sung Jae Kim](#)
- 15:00 **Electroconvection instability and deionization shock in a circular microchannel**
» [Prof. Daosheng Deng](#)
- 15:30 **A Review of Ionic-Liquid Electrospray Propulsion and Related Electrokinetic Phenomena**
» [Mr. Louis Perna](#), [Prof. Paulo Lozano](#)
- 15:45 **Coffee Break**
Ting Foyer (E51)
- 16:00 **Mathematical Modeling (C2)**
Wong Auditorium (E51-115)
Chaired by: [Prof. Boris Zaltzman](#)
- 16:00 **On the scale dependence of flow structures and transport in electroconvection near ion-selective membranes**
» [Prof. Ali Mani](#), [Ms. Karen Wang](#)
- 16:30 **Electrokinetic Control of Viscous Fingering**
» [Dr. Mohammad Mirzadeh](#), [Dr. Tao Gao](#), [Prof. Martin Bazant](#)
- 16:45 **From Electrodiffusion Theory to the Electrohydrodynamics of Leaky Dielectrics through the Weak Electrolyte Limit**
» [Prof. Yoichiro Mori](#), [Dr. Yuan Young](#)
- 17:00 **Particle rotation driven systems**
» [Prof. Andrejs Cebers](#)

- 17:15 **Fluctuating hydrodynamics of electrolytes at electroneutral scales**
» [Prof. Aleksandar Donev](#)

- 17:30 **Oscillating Electric Fields in Liquids Create a Long-Range Steady Field: Implications for Electrokinetics**
» [Mr. S. M. H. Hashemi Amrei](#), [Dr. Scott Bukosky](#), [Prof. Greg Miller](#), [Prof. William Ristenpart](#)

Thursday, 13 June

- 8:00 **Registration**
Tang Center Entrance (E51)
- 9:00 **Keynote Lecture (K2)**
Wong Auditorium (E51-115)
Chaired by: [Prof. Martin Bazant](#)
- 9:00 **Metamaterials, Plasmonics and Electrochemistry: Tuning photonic functionalities in real time**
» [Prof. Alexei Kornyshev](#)
- 9:45 **Ionic Liquids (S2)**
Wong Auditorium (E51-115)
Chaired by: [Prof. Rui Qiao](#)
- 9:45 **Unexpected surface forces generated by the action of electric fields across ionic liquid electrolytes**
» [Dr. Carla Perez Martinez](#), [Prof. Susan Perkin](#)
- 10:00 **Free and Bound States of Ions in Ionic Liquids, Conductivity, and Underscreening Paradox**
» [Prof. Guang Feng](#), [Mr. Ming Chen](#), [Mr. Sheng Bi](#), [Mr. Zachary Goodwin](#), [Prof. Eugene Postnikov](#), [Prof. Nikolai Brilliantov](#), [Prof. Michael Urbakh](#), [Prof. Alexei Kornyshev](#)

Continued from **Thursday, 13 June**

10:15 **Charge Screening and Electrokinetic Phenomena with Strongly Correlated Ions**
» Mr. Amir Levy, Mr. Pedro de Souza, Mr. Michael McEldrew, Prof. Martin Bazant

10:45 **Coffee Break**
Ting Foyer (E51)

11:00 **Keynote Lecture (K3)**
Wong Auditorium (E51-115)
Chaired by: Prof. Martin Bazant

11:00 **Electrokinetics of complex interfaces: from metals, hydrogels to bacteria**
» Prof. Jerome F.L. Duval, Prof. Herman P. Van Leeuwen

11:45 **Poster Soundbites (PS2)**
Wong Auditorium (E51-115)

11:45 **A novel electrochemical flow sensor using the convective-diffusive ionic concentration layer by ionic concentration-polarization**
» Dr. Sinwook Park, Dr. Ramadan Abu-Rjal, Prof. Gilad Yossifon

11:50 **Diffusiophoretic migration of colloids induced by freely falling soluto-inertial beacons**
» Mr. Anirudha Banerjee, Prof. Todd Squires

11:55 **Electrodynamics of particle compaction in electronic ink**
» Mr. Bavo Robben, Prof. Filip Beunis, Prof. Kristiaan Neyts, Dr. Robert Fleming, Mr. Bram Sadlik, Dr. Thomas Johansson, Dr. Lorne Whitehead, Prof. Filip Strubbe

12:00 **Does Current Monitoring work for Nanochannels with thick electrical double layers?**
» Mr. Siyang Xiao, Dr. Quan Xie, Mr. Zachary Wollman, Dr. Chuanhua Duan

12:05 **Electrorotation of semiconducting microspheres**
» Ms. Laida Rodríguez-Sánchez, Prof. Antonio Ramos, Prof. Pablo García-Sánchez

12:10 **Non-uniform electro-osmotic flow drives elastic deformation instability**
» Mr. Evgeniy Boyko, Mr. Ran Eshel, Prof. Amir Gat, Prof. Moran Bercovici

12:15 **Electrokinetic flows on nanostructured superhydrophobic surfaces**
» Mr. aktaruzzaman al hossain, Dr. Antonio Checco, Dr. Carlos Colosqui

12:20 **Overlapping double layer effects on electrokinetic squeezing flow electrical power generation**
» Prof. Hsin-Fu Huang, Mr. Shi-Wei Jian, Mr. Yung-Cheng Cheng

12:30 **Poster & Lunch (P2)**
Walker Memorial (50, Main Hall)

1 A novel electrochemical flow sensor using the convective-diffusive ionic concentration layer by ionic concentration-polarization
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3 Electrodynamics of particle compaction in electronic ink
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4 Does Current Monitoring work for Nanochannels with thick electrical double layers?
» Mr. Siyang Xiao, Dr. Quan Xie, Mr. Zachary Wollman, Dr. Chuanhua Duan

Continued from **Thursday, 13 June**

- # 5 Electrorotation of semiconducting microspheres**
» Ms. Laida Rodríguez-Sánchez, Prof. Antonio Ramos, Prof. Pablo García-Sánchez

- # 6 Non-uniform electro-osmotic flow drives elastic deformation instability**
» Mr. Evgeniy Boyko, Mr. Ran Eshel, Prof. Amir Gat, Prof. Moran Bercovici

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- # 8 Overlapping double layer effects on electrokinetic squeezing flow electrical power generation**
» Prof. Hsin-Fu Huang, Mr. Shi-Wei Jian, Mr. Yung-Cheng Cheng

- # 9 Sedimentation of Charge-Regulating Porous Particles**
» Mr. Chien-Yu Lin, Prof. Huan J. Keh

- # 10 Electrohydrodynamic scaling laws analysis in a microfluidic isoDEP device**
» Mr. mohamed zakarya Rashed, Ms. Grason Gasser, Mr. Lincoln Curry, Dr. Stuart Williams

- # 11 Molecular dynamics study of nanostructure formation of imidazolium-based ionic liquids with long-alkyl chains**
» Dr. Hayato Shiba, Prof. Hailong Peng, Prof. Momoji Kubo

- # 12 Graphitic Carbon Nitride Impregnated Niobium oxide (g-C₃N₄/Nb₂O₅) Type (II) Heterojunctions and its Synergetic Solar-Driven Hydrogen Generation**
» Dr. Ibrahim M. Zarin, Prof. Ahsanulhaq Qurashi, Dr. Nadeem Baig

- # 13 Modeling of Direct Current Electrokinetic Motion of Janus Particles and Droplets**
» Mr. Atakan Atay, Prof. Barbaros Cetin, Prof. Ali Beskok

- # 14 DIFFUSION-BASED SEPARATION USING BIDIRECTIONAL ELECTROOSMOTIC FLOW**
» Ms. Vesna Bacheva, Dr. Federico Paratore, Dr. Shimon Rubin, Dr. Govind Kaigala, Prof. Moran Bercovici

- # 15 Electrokinetic trapping of anisotropic particles**
» Prof. Filip Strubbe, Mr. Bavo Robben, Dr. John Puthenparampil George, Ms. Ingrid Amer Cid, Prof. Filip Beunis, Prof. Kristiaan Neyts

- # 16 Temperature dependence of Diffusiophoresis**
» Mr. Parth Shah, Dr. Huanshu Tan, Mr. David Taylor, Mr. Anirudha Banerjee, Dr. Xiaoyu Tang, Dr. Nan Shi, Dr. Afnan Mashat, Dr. Amr Abdel-Fattah, Prof. Todd Squires

- # 17 Electroosmotic flow over superhydrophobic surfaces**
» Mr. Baruch Rofman, Mr. Sebastian Dehe, Prof. Steffen Hardt, Prof. Moran Bercovici

- # 18 Nanopore Electrokinetic Tweezer for single nanoparticle characterization/ manipulation.**
» Mr. Rami Yazbeck, Dr. Mohammad Amin Alibakhshi, Mr. Joseph Von Schoppe, Dr. Kamil Ekinci, Dr. Chuanhua Duan

- # 19 Optimized Coagulation Pathway of Al₁₃: Effect of In-situ Aggregation of Al₁₃**
» Prof. Dongsheng Wang, Dr. Guangyu An, Mrs. Pin Wang

- # 20 Effect of the double layer structure on the photo-induced charge transfer across the interface between two immiscible liquids**
» Mr. Andres Molina, Dr. Micheal Scanlon

- # 21 Continuous Diffusiophoretic Nanoparticle Separation by Enhanced Ion Exchange**
» Mr. Myungjin Seo, Prof. Sung Jae Kim, Prof. Hyomin Lee, Mr. Sungmin Park, Mr. Dokeun Lee

Continued from **Thursday, 13 June**

- # 22 **Electroneutrality breakdown in nanopores: a 1d mean-field theory**
» Mr. Amir Levy, Prof. Martin Bazant
 - # 23 **Electrostatic and density correlations in the electrical double layer**
» Mr. Pedro de Souza, Prof. Martin Bazant
 - # 24 **Ion Association vs Ion Solvation and the Electrical Double Layer in Water-in-Salt Electrolytes**
» Mr. Michael McEldrew, Mr. Zachary A. H. Goodwin, Mr. Sheng Bi, Prof. Alexei Kornyshev, Prof. Martin Bazant
 - # 25 **Charge trapping at hydrophobic polymer-electrolyte interfaces enables efficient drop-based energy harvesting**
» Ms. Hao Wu, Mr. Niels Mendel, Dr. Arun Banpurkar, Dr. Dirk van den Ende, Prof. Guofu Zhou, Prof. Frieder Mugele
 - # 26 **Manipulating the Belousov-Zhabotinsky reaction with silver-silver bromide electrodes**
» Mr. Arnaldo Rodriguez-Gonzalez, Prof. Brian Kirby
 - # 27 **Red-ox Responsive Hydrogel**
» Dr. Baptiste Blanc, Prof. Zhenkhun Zhang, Prof. Bing Xu, Prof. Hyunmin Yi, Prof. Seth Fraden
 - # 28 **Single charging events on colloidal particles in a nonpolar liquid with surfactant**
» Prof. Filip Beunis, Dr. Caspar Schreuer, Mr. Bavo Robben, Prof. Filip Strubbe, Prof. Kristiaan Neyts
- 14:00 **Microfluidics (C3)**
Wong Auditorium (E51-115)
Chaired by: Prof. Juan Santiago
- 14:00 **Microslit Electrokinetic Analyses to Explore Soft Macroscopic Interfaces**
» Prof. Ralf Zimmermann, Prof. Carsten Werner

- 14:30 **Dynamic Flow Patterning with Localized Field Effect Electroosmosis**
» Dr. Federico Paratore, Ms. Vesna Bacheva, Dr. Govind Kaigala, Prof. Moran Bercovici
- 14:45 **Active electrokinetic control of the concentration-polarization layer in a microchannel-ion-permselective membrane system**
» Prof. Gilad Yossifon, Dr. Sinwook Park
- 15:00 **Electrokinetic microflow of non-Newtonian solutions in polyelectrolyte brush-grafted channels**
» Dr. Byoungjin Chun, Prof. Myung-Suk Chun, Dr. Tae-Seok Lee
- 15:15 **AC electrokinetics in a deterministic-lateral-displacement device**
» Mr. Victor Calero, Prof. Pablo García-Sánchez, Prof. Antonio Ramos, Prof. Hywel Morgan
- 15:45 **Coffee Break**
Ting Foyer (E51)
- 16:00 **Colloids and Interfaces (C4)**
Wong Auditorium (E51-115)
Chaired by: Prof. Jerome F.L. Duval
- 16:00 **Ion adsorption, hydration, and the structure of the electric double layer: classical ideas and recent insights from high resolution Atomic Force Microscopy**
» Prof. Frieder Mugele
- 16:30 **Structure and Dynamics of Electrical Double Layers in Thin Brine Films**
» Mr. Chao Fang, Prof. Rui Qiao
- 16:45 **Effect of Specific ions on the Reduction of Interfacial Tension by Ionic Surfactants**
» Dr. Vinay Raman, Dr. Hooisweng Ow, Mr. Gawain Thomas, Dr. Michael Szulczewski, Dr. Ali Dogru

Continued from **Thursday, 13 June**

- 17:00 **Flow-Induced Surface Charge Heterogeneity in Electrokinetics due to Stern-Layer Conductance Coupled to Reaction Kinetics**
» Prof. Rene van Roij, Mr. Ben Werkhoven, Dr. Jeffrey Everts
- 17:15 **AC electrokinetics of salt-free, multilayered soft particles**
» Dr. Ángel V. Delgado, Dr. Felix Carrique, Ms. Sara Bermudez, Dr. María L. Jiménez, Dr. Silvia Ahualli
- 18:30 **Conference Banquet**
Media Lab (E14, 6th floor)

Friday, 14 June

- 8:00 **Registration**
Tang Center Entrance (E51)
- 9:00 **Bio-electrokinetics (C5)**
Wong Auditorium (E51-115)
- 9:00 **Holistic molecular imaging and rapid phenotyping of complex biological systems**
» Prof. Kwanghun Chung
- 9:30 **Spatio-temporal morphogen gradients to direct cell-fate decisions in glycosaminoglycan-based hydrogels**
» Prof. Ralf Zimmermann, Dr. Felix Schrön, Dr. Yanuar D. P. Limasale, Dr. Christoph Hentschel, Dr. Passant Atallah, Dr. Uwe Freudenberger, Prof. Carsten Werner
- 9:45 **Electric Field Driven Characterization of Biovesicles**
» Prof. Prashanta Dutta, Mr. Adnan Morshed
- 10:00 **DNA thermal stability depends on solvent viscosity**
» Dr. Nancy Stellwagen

- 10:15 **Propulsion of asymmetric dielectric particles under high frequency AC electric fields**
» Mr. Xingfu Yang, Dr. Jingjing Gong, Prof. Ning Wu

- 10:30 **Interpretation of the effect of particle size on fast aggregation rate using structural layer model**
» Dr. Hongyan Sun, Prof. Daosheng Deng

- 10:45 **Coffee Break**
Ting Foyer (E51)

- 11:00 **Keynote Lecture (K4)**
Wong Auditorium (E51-115)
Chaired by: Dr. Mohammad Mirzadeh

- 11:00 **Capacitive deionization of water: Resonance and selective extraction**
» Dr. Ashwin Ramachandran, Mr. Diego Oyarzun, Prof. James Palko, Dr. Steven Hawks, Dr. Patrick Campbell, Dr. Michael Stadermann, Prof. Juan Santiago

- 11:45 **Poster Soundbites (PS3)**
Wong Auditorium (E51-115)

- 11:45 **Study of Ion Transport Through A Two-Dimensional Porous Charged Interface**
» Mrs. Mandakranta Ghosh, Mr. Koen F. A. Jorissen, Dr. Jeffery Wood, Prof. Rob Lammertink

- 11:50 **Theory of coupled ion transport and chemical conversions in bioelectrochemical systems**
» Mr. Aymar de Lichtervelde, Dr. Maarten Biesheuvel, Dr. Hubertus V. M. Hamelers, Dr. Annemiek ter Heijne, Dr. Jouke Dykstra

- 11:55 **Theory of electrokinetic transport in deformable nanochannels**
» Mr. Mpumelelo Matse, Prof. Peter Berg, Prof. Michael Eikerling

Continued from Friday, 14 June

- 12:00 **Dielectrophoresis Based Characterization of LEA Proteins**
» Mr. mohamed zakarya Rashed, Mr. Clinton Belott, Dr. Michael Menze, Dr. Stuart Williams
- 12:05 **Hydrodynamics and adhesion of a lipid bilayer membrane under an electric field**
» Dr. Yuan Young, Dr. Bryan Quaife, Dr. Carlos Colosqui
- 12:10 **The Role of Thermal Voltage in Biology**
» Prof. James Sterling
- 12:15 **CFD simulations of electrokinetic instabilities in electromembrane processes**
» Ms. Mariagiorgia La Cerva, Dr. Michele Tedesco, Prof. Michele Ciofalo, Prof. Giorgio Micale
- 12:20 **Extending the Taylor-Aris dispersion model to electro-osmotically driven Hele-Shaw flows**
» Mr. Sebastian Dehe, Ms. Imke Lorenz, Prof. Steffen Hardt
- 12:25 **Theoretical and experimental investigations of self-similar interfacial impedance of disk electrodes in high conductivity media**
» Mr. Anil Koklu, Mr. Amin Mansoorifar, Prof. Vladimir Ajaev, Prof. Ali Beskok
- 12:30 **Poster & Lunch (P3)**
Walker Memorial (50, Main Hall)

- # 1 Study of Ion Transport Through A Two-Dimensional Porous Charged Interface**
» Mrs. Mandakranta Ghosh, Mr. Koen F. A. Jorissen, Dr. Jeffery Wood, Prof. Rob Lammertink

- # 2 Theory of coupled ion transport and chemical conversions in bioelectrochemical systems**
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- # 3 Theory of electrokinetic transport in deformable nanochannels**
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- # 4 Dielectrophoresis Based Characterization of LEA Proteins**
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- # 5 Hydrodynamics and adhesion of a lipid bilayer membrane under an electric field**
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- # 6 The Role of Thermal Voltage in Biology**
» Prof. James Sterling
- # 7 CFD simulations of electrokinetic instabilities in electromembrane processes**
» Ms. Mariagiorgia La Cerva, Dr. Michele Tedesco, Prof. Michele Ciofalo, Prof. Giorgio Micale
- # 8 Extending the Taylor-Aris dispersion model to electro-osmotically driven Hele-Shaw flows**
» Mr. Sebastian Dehe, Ms. Imke Lorenz, Prof. Steffen Hardt
- # 9 Theoretical and experimental investigations of self-similar interfacial impedance of disk electrodes in high conductivity media**
» Mr. Anil Koklu, Mr. Amin Mansoorifar, Prof. Vladimir Ajaev, Prof. Ali Beskok
- # 10 Parallelized Electrorotation in single cell DEP micro cages**
» Mr. Kevin Keim, Mr. Mohamed Z Rashed, Prof. Carlotta Guiducci

Continued from Friday, 14 June

- # 11 **Chemically modified activated carbon for high performance capacitive deionization**
» Mr. Oneeb Haq
- # 12 **Electrokinetic Scanning Probe for Localized Surface Patterning and Analysis**
» Ms. Nadya Ostromohov, Prof. Moran Bercovici, Dr. Govind Kaigala
- # 13 **Do We Need to Pose a Closure Problem to Capture the Dynamics of the Capacitive Charging of Porous Electrodes?**
» Mr. Amit Naftali Shocron, Prof. Matthew E. Suss
- # 14 **Self-similar interfacial impedance of electrodes in high conductivity media**
» Mr. Anil Koklu, Mr. Amin Mansoorifar, Prof. Vladimir Ajaev, Prof. Ali Beskok
- # 15 **Theoretical Analysis of Electrochemically Mediated Selective Adsorption for Water Treatment**
» Ms. Fan He, Prof. Martin Bazant, Prof. T. Alan Hatton
- # 16 **Direct determination of the electrophoretic mobility of individual micro- and nanoparticles**
» Ms. Ingrid Amer Cid, Prof. Kristiaan Neyts, Prof. Filip Strubbe
- # 17 **Low dispersion flow cell with asymmetric redox active electrodes for selective removal of ionic pollutants**
» Dr. ALI HEMMATIFAR, Mr. Kai-Jher Tan, Prof. T. Alan Hatton
- # 18 **Thermodynamics of signal conduction in neurons**
» Mr. Aymar de Lichtervelde, Mr. Pedro de Souza, Prof. Martin Bazant
- # 19 **Theory of freezing point depression and freeze-thaw damage by nano-fluidic salt trapping**
» Dr. Tingtao Zhou, Dr. Mohammad Mirzadeh, Dr. Roland Pelleng, Prof. Martin Bazant

- # 20 **Self-Charging Dielectric Elastomers**
» Prof. Thiago Burgo, Prof. Fernando Galembeck, Dr. Leandra P. Santos, Ms. Kelly Moreira
- # 21 **Mass transport through an annular microchannel by an oscillatory electroosmotic flow of a Maxwell fluid**
» Dr. Oscar Bautista, Dr. Manuel Peralta, Dr. Federico Méndez
- # 22 **Viscoelectric Effects in an oscillatory electro-osmotic flow with slippage condition**
» Mr. Rubén Darío Baños, Dr. JOSE CARLOS ARCOS, Dr. Eric Gustavo Bautista
- # 23 **The kinetics of jet impingement-induced HeLa cell detachment from graphene and graphene oxide**
» Prof. Lubomir Lapcik, Mr. Jakub Vlcek, Dr. Barbora Lapcikova, Prof. Michal Otyepka
- # 24 **Ion Transport and Current Rectification in Nanopores Subject to Dual pH-Gradient and Voltage Bias**
» Ms. Tsai-Wei Lin, Prof. Jyh-Ping Hsu, Dr. Chih-Yuan Lin, Prof. SHIOJENN TSENG
- # 25 **Electrokinetic Ion Transport in an Asymmetric Double-gated Nanochannel**
» Prof. SHIOJENN TSENG, Prof. Jyh-Ping Hsu
- # 26 **Thermodynamics of soil electrokinetic treatment**
» Dr. EMIGDIA GUADALUPE SUMBARDA RAMOS, Dr. MERCEDES OROPEZA GUZMAN, Dr. IGNACIO GONZALEZ MARTINEZ, Dr. MARGARITA TEUTLI LEON, Dr. Bayardo Murillo Rivera
- # 27 **Theoretical analysis on the influence of viscous effects on the acoustophoretic trapping**
» Mr. Carlos Vargas, Dr. Ivan Campos

14:00

Physics of Membranes (S3)

Wong Auditorium (E51-115)

Chaired by: Prof. Victor Nikonenko

Continued from **Friday, 14 June**

- 14:00 **Next-Generation Desalination Membranes**
» Prof. Menachem Elimelech
- 14:30 **Chronopotentiometry of heterogeneous ion-exchange membranes with hydrophobic or hydrophilic non-conductive surface areas: 2D simulation**
» Dr. Semyon Mareev, Mr. Andrey Nebavskiy, Prof. Victor Nikonenko
- 14:45 **Theory of ion and water transport in electron-conducting membrane pores with pH-dependent chemical charge**
» Dr. Li Zhang, Dr. Maarten Biesheuvel, Prof. Ilya Ryzhkov
- 15:00 **Understanding coion transport and water dissociation in bipolar electrodialysis for energy storage applications**
» Dr. Michele Tedesco
- 15:15 **1D and 2D modeling of electrodialysis and reverse osmosis**
» Dr. Maarten Biesheuvel
- 15:30 **Electrokinetic enhancement of ion transport through changing membrane topology**
» Dr. Anne Benneker, Dr. Burcu Gumuscu, Mr. Ernest Derckx, Prof. Rob Lammertink, Prof. Jan Eijkel, Dr. Jeffery Wood
- 15:45 **Coffee Break**
Ting Foyer (E51)
- 16:00 **Physics of Membranes (S4)**
Wong Auditorium (E51-115)
Chaired by: Dr. Maarten Biesheuvel
- 16:00 **Faradaic Modulation of Redox Polymer-Functionalized Electrodes for Controlled Electrosorption**
» Mr. Sahag Voskian, Ms. Fan He, Prof. T. Alan Hatton

- 16:30 **Shock Electrodialysis for Ion-Selective Water Purification**
» Dr. Kameron Conforti, Mr. Mohammad Alkhadra, Dr. Tao Gao, Ms. Huanhuan Tian, Prof. Martin Bazant
- 16:45 **Mechanisms of ion transport in nanopores with conductive walls: new mathematical models and experimental results**
» Prof. Ilya Ryzhkov, Mr. Anton Vyatkin, Ms. Anastasia Bortsova, Dr. Mikhail Simunin
- 17:00 **Theory of simultaneous desalination and electricity generation via an electrodialysis cell driven by spontaneous redox reactions**
» Mr. Imri Atlas, Prof. Matthew E. Suss
- 17:15 **Fabrication of Antifouling Electroconductive Thin Film Composite Membranes**
» Mr. Amin Karkooti, Dr. Masoud Rastgar, Prof. Mohtada Sadrzadeh, Prof. Neda Nazemifard
- 17:30 **Conference Closing & Poster Awards**
Wong Auditorium (E51-115)

Temperature-gradient-induced electrokinetic transport of electrolyte solutions in charged capillaries

Authors

Mr. Wenyao Zhang - Xi'an Jiaotong University

Prof. Qiuwang Wang - Xi'an Jiaotong University

Prof. Min Zeng - Xi'an Jiaotong University

Prof. Cunlu Zhao - Xi'an Jiaotong University

Abstract

We present a theoretical study of temperature-gradient-induced electrokinetic transport of electrolyte solutions in a charged micro/nanocapillary. The study is based on a semi-analytical model developed by simultaneously solving the non-isothermal Poisson-Nernst-Planck/Navier-Stokes equations with the lubrication approximation. The semi-analytical model is shown to be governed by eight parameters, including two temperature-related parameters (temperature and its gradient), two electro-kinetic parameters (ζ potential of capillary and the ratio of capillary radius to the Debye length $\kappa_0 a$) and four physical properties relevant to cation and anion (i.e., Soret coefficient difference ΔS_T , average Soret coefficient S_T , normalized difference in diffusivities χ and Péclet number λ). This paper reveals the interplay and relative importance of the thermoelectric mechanism due to (a) the convective transport of ions caused by the fluid flow, (b) the dependence of ion electrophoresis on temperature, (c) the difference in the Soret coefficients of cation and anion. The second thermoelectric effect is dominant for high ζ potentials with vary small $\kappa_0 a$, while the last is dominant for low ζ potentials or very large $\kappa_0 a$. Moreover, the last two thermoelectric effects can cooperate or counteract depending on the sign of $\zeta \Delta S_T$. Finally the temperature-gradient-induced electrokinetic flow is found to be the competition or cooperation of an electroosmotic flow component due to the thermoelectric field and a thermoosmotic flow component due to combined effects of the excess osmotic pressure gradient and dielectric body force. These two flow components may cooperate with or cancel each other depending on ζ and $\kappa_0 a$.

The results are beneficial for understanding the temperature-gradient-induced electrolyte transport in charged capillaries, and also pave a way for the designs of low-grade waste heat recovery devices and thermo-electroosmotic pump.

Routine, ensemble characterisation of zeta potential in saturated ionic strengths

Authors

Dr. Jason Corbett - Malvern Panalytical Ltd

Mr. Jake Austin - Malvern Panalytical Ltd

Dr. Diogo Fernandez - Malvern Panalytical Ltd

Abstract

With the pervasive incursion of manufactured nano-particles into the environment, the need to characterise pharmaceuticals and living systems in replicated *in vivo* conditions, the continuing development of new theories to describe the electrokinetic behaviour of nano-particles in representative ionic strengths and numerous other applications, there is an urgent requirement to provide simple and effective experimental tools to validate these models and explore new systems. Micro-electrophoresis implemented with a diffusion barrier, which isolates the dispersed phase from the electrode surface, is demonstrated as enabling for such measurements, preventing the catastrophic denaturation, out-gassing and precipitation observed when the dispersed phase is in close proximity to the electrode surface. Using a simple and precise measurement of a few minutes duration and a disposable cell in a standard laboratory light scattering instrument, we reproduce the theoretically predicted phenomena of asymptotic, non-zero zeta potential and charge inversion, with increasing ionic strength. We also explore the direct and indirect Hofmeister series dependency and present a new result: a decreasing variation in zeta potential with *pH* as molarity increases. An SOP is developed and described to encourage further work

Hydrodynamics and adhesion of a lipid bilayer membrane under an electric field

Authors

Dr. Yuan Young - New Jersey Institute of Technology

Dr. Bryan Quaife - Florida State University

Dr. Carlos Colosqui - Stony Brook University

Abstract

Phospholipid bilayer membranes have been widely utilized as mimics of biological cell membranes in biophysics and material engineering. Many applications of lipid bilayer membranes involve both electrohydrodynamics and adhesion to a structure under an electric field. Steinkuhler et al. (Biophys. J., 2016) illustrated how vesicle adhesion on an ITO surface can be modulated by an electric field. Once on the substrate, the flow around the adhered vesicle due to an imposed external flow has been investigated in the context of transmission of stress in cells (Sebastian et al, J. Chem. Phys., 2017). In this work we study the effects of adhesion on vesicle hydrodynamics by using the state-of-the-art boundary integral simulations. We also investigate how the adhesion effects may depend on the osmotic pressure when the separation distance (between two membranes or membranes and solid) is less than the Debye length, the scale of the electric double layer (EDL). For example, the draining of the thin film between two vesicle membranes depends on the overlap of the EDL. We illustrate how the scaling of the draining time may depend on the details of EDL. We also quantify the adhesion effects on electrohydrodynamics of a lipid bilayer membrane (either a supported lipid bilayer (SBL) or a suspended vesicle in close vicinity of another vesicle).

DNA thermal stability depends on solvent viscosity

Authors

Dr. Nancy Stellwagen - University of Iowa

Abstract

Free solution capillary electrophoresis (CE) is a useful tool to characterize the physicochemical properties of DNA. Here, we have used CE to determine the effect of monovalent cation size on DNA thermal stability, using hairpins with 6 base pair stems and 4 nucleotide loops as the reporter system. The melting temperatures observed in buffers containing Na^+ ions were 17°C higher than observed in buffers containing the same concentration of tetrabutylammonium (TBA^+) ions, regardless of sequence, indicating that TBA^+ exerts a through-solvent effect on DNA thermal stability. In addition, the melting temperatures observed for the hairpins decreased linearly with increasing solvent viscosity when the viscosity was modified by changing the size of the alkyl side chains in the tetraalkylammonium ions. The normalized melting temperatures of the hairpins agreed with literature data of the normalized melting temperatures of another small DNA hairpin, a small RNA duplex, and sonicated calf thymus DNA in tetraalkylammonium ion buffers.

Mass transport through an annular microchannel by an oscillatory electroosmotic flow of a Maxwell fluid

Authors

Dr. Oscar Bautista - Instituto Politécnico Nacional

Dr. Manuel Peralta - Instituto Politécnico Nacional

Dr. Federico Méndez - Universidad Nacional Autónoma de México

Abstract

In this work, we theoretically analyze the mass transfer in a micro-annulus with symmetric and asymmetric wall zeta potentials driven by an oscillatory electroosmotic flow (OEOF) of a Maxwell fluid. The micro-annulus connects two reservoirs having different concentrations of an electro-neutral solute. To analyze the hydrodynamic and mass transport in the OEOF we combine the linear Maxwell viscoelastic model, the Cauchy equation, and the electric field solution obtained from the linearized Poisson-Boltzmann equation, yielding an expression for momentum in terms of the velocity field, allowing to determine

the hydrodynamic field, which is used in the species conservation equation to obtain the mass concentration, and accordingly, the mass transport through the micro-annulus. The mass transfer is controlled by dimensionless parameters: an angular Reynolds number, the ratio of the zeta potentials of the micro-annulus walls, the electrokinetic parameter, the gap between the two cylinders, the Schmidt number and the elasticity number. The results indicate that the velocity and concentration distributions across the micro-annulus become non-uniform as the angular Reynolds number increases. It is also revealed that a suitable combination of the elasticity number and the gap between the two cylinders, the total mass transfer rate can be increased.

Viscoelectric Effects in an oscillatory electro-osmotic flow with slippage condition

Authors

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Dr. JOSE CARLOS ARCOS - Instituto Politécnico Nacional. ESIME unidad Azcapotzalco

Dr. Eric Gustavo Bautista - Instituto Politécnico Nacional. ESIME unidad Azcapotzalco

Abstract

The flow structure in an oscillatory electroosmotic flow (OEF) through a microchannel is studied numerically by considering that the viscosity of the fluid is a well-defined function of the double layer field strength. The concentration of a passive solute in the OEF which is in a periodical state for a newtonian fluid through a microchannel was determined by the convection-diffusion equation assuming an initial linear distribution of the concentration of solute along the microchannel. Flow is considered fully developed hydrodynamically in the axial direction. To generate an oscillatory flow, at the ends of the microchannel there is a cathode and an anode through which an electric field

that has a sinusoidal behavior is applied, and this induces the oscillatory movement in the fluid. The governing equations for the hydrodynamic were simplified and solved in the limit of the lubrication theory. On the other hand, the Navier-slip boundary condition at the interface between the microchannel walls and the fluid is considered, which is a general condition that has the no-slip condition as a limit case. In addition, these walls are subject to a surface electrical potential larger than 0.025V, so the Debye-Hückel approximation was not applied. The microchannel is connected at its ends to two containers that are at a constant concentration of the solute, where the concentration of the left end is higher than the right end, the electrolyte contained in the microchannel is considered symmetric and is not affected by any electric potential. Our results suggest that the viscoelectric effect, the slippage condition and the Womersley control the behavior of the OEF increasing the velocity of the fluid in comparison when the slippage condition is absent. On the other hand, the concentration of a non-reacting solute was solved by the convection-diffusion equation assuming an initial linear distribution of the concentration of the solute.

Electrokinetic instability at an extremely non-equilibrium electrophoresis of ion-selective microparticle

Authors

Ms. Elizaveta Frants - Kuban State University, Financial University, University of Bordeaux

Dr. Georgy Ganchenko - Financial University

Dr. Vladimir Shelistov - Financial University

Dr. Sakir Amiroudine - University of Bordeaux

Dr. Evgeny Demekhin - Financial University

Abstract

Electrophoresis of an ion-selective microparticle in a binary diluted electrolyte solution is considered for a strong applied electric field. When ions pass through an ion-selective spherical particle, three boundary layers, that are nested inside each other, are formed at the front of the particle in the region of incoming ion flux: an electric double layer (EDL), a space charge region (SCR) and a thin diffusion layer. Near the surface of the outgoing ion flux (formed only by the EDL), a region of the enriched electrolyte with a strong concentration gradient emerges. Increasing the magnitude of the external electric field makes this enriched electrolyte region narrower, and its conductivity increases. At some critical value of the electric field, the steady-state solution loses stability and the system becomes unstable. However, depending on the Debye number, this instability manifests itself in different regions. For small Debye numbers, it takes place in the SCR at the forefront of the particle, and for larger values, it originates at the poles and propagates towards the equator at the backside of the particle corresponding to the outgoing ion flux. This instability affects the outgoing stream of the enriched electrolyte with high electrical conductivity.

For the instability in the SCR, two kinds of microvortices are found: large steady Dukhin-Mishchuk vortices, and small vortices issued from electrokinetic instability that propagate from the incoming-flux equator of the particle towards the Dukhin-Mishchuk vortices near the poles. A jet of enriched electrolyte appears on the backside of the sphere. With the increase in the Debye number small vortices disappear, but Dukhin-Mishchuk vortices are still present and they become highly unsteady. These unsteady Dukhin-Mishchuk vortices perturb the electric conductivity jet behind the sphere, and so this jet becomes unstable.

The problem has been treated both by numerical and analytical approaches. For small EDL thickness and sufficiently high electric fields (the case of overlimiting currents), a semi-analytical analysis based on linear stability analysis of the steady-state 1D solution has been performed. This analysis has been complemented by DNS of the nonstationary Nernst-Planck-Poisson-Stokes

system, with the corresponding boundary and initial conditions. The results from DNS and semi-analytical solutions were successfully compared in terms of electric potential drop and the length of SCR or the ion flux at different points of the granule surface. The experimental electroosmotic velocity (at the limit of SCR region) and the electrophoretic velocity are also in a reasonably good agreement with our theory. Moreover, our results have improved the discrepancy with experiments of the Dukhin's relation. The stability diagram in terms of critical electric field as a function of Debye number shows the transition of the two regimes described above.

Electrokinetics of complex interfaces: from metals, hydrogels to bacteria

Authors

Prof. Jerome F.L. Duval - CNRS

Prof. Herman P. Van Leeuwen - Wageningen University

Abstract

Hans Lyklema's contributions in the field of interface and colloid science have undeniably impacted on generations of scientists active in fields as diverse as electrokinetics, electric double layer analysis under equilibrium and dynamic conditions, polymer/ion/polyelectrolyte adsorption at surfaces, dynamics of proteins at interfaces, interfacial rheology, as well as in domains of both practical and fundamental relevance such as food emulsions and cell adhesion. If a common point were to be found between all these apparently well-differentiated themes, that would certainly be the importance of interfacial charges and ensuing electrostatics in setting the reactivity of molecular or colloidal systems in aqueous solutions, may they be ions, micelles, minerals, metals or microbes. For many years to come, Hans' work shall remain decisive in bridging various branches of colloid science and other related fields, and in educating the younger (and older) generations with interests in colloid and interface sciences. For that purpose, Hans has left us a formidable heritage in the form of 5 volumes 'Fundamentals of Interface and Colloid Science'. As a tribute to Hans' work that touched upon so many aspects of properties and

reactivity of interfaces, this presentation shall modestly focus on the electrokinetic properties of (i) metallic surfaces depolarized by (bipolar) faradaic electron transfer processes, (ii) soft zwitterionic interfaces and (iii) bacteria. All have in common that interpretation of their electrokinetic features requires the account of generic conductivity terms stemming from the transports of electrons (i), ions and fluid (ii/iii) within the considered material. Applications within the framework of bipolar electrochemical detection of chemicals, bacterial adhesion or evaluation of the toxicity of dispersed nanoparticles toward bacteria will be invoked.

Sedimentation of Charge-Regulating Porous Particles

Authors

Mr. Chien-Yu Lin - Department of Chemical Engineering, National Taiwan University

Prof. Huan J. Keh - Department of Chemical Engineering, National Taiwan University

Abstract

The sedimentation of a charge-regulating porous sphere surrounded by an arbitrary electric double layer, that usually models a permeable polyelectrolyte coil or aggregate of nanoparticles, is analyzed. The hydrodynamic frictional segments and ionogenic functional groups uniformly distribute in the porous sphere, and a regulation mechanism for the dissociation and association reactions occurring at these functional groups linearly relates the local electric potential to fixed charge density. The linearized electrokinetic equations governing the ionic concentration (or electrochemical potential energy), electric potential, and fluid velocity fields are solved for the case of a small basic fixed charge density by a regular perturbation method. Analytical formulas for the sedimentation velocity of a porous sphere and sedimentation potential of a dilute suspension of porous spheres are then obtained. The charge regulation tends to reduce the electrokinetic retardation to sedimentation velocity and the sedimentation potential (can be as much as 50 and 25 per cents, respectively) compared to the case that the fixed charge density is a constant. Both the

electrokinetic retardation to sedimentation velocity and the sedimentation potential vanish at the isoelectric point of the particles. The increase in the bulk concentration of the potential-determining ions crossing the isoelectric point changes signs of the fixed charges and thus causes a reversal in the direction of the sedimentation potential.

Oscillating Electric Fields in Liquids Create a Long-Range Steady Field: Implications for Electrokinetics

Authors

Mr. S. M. H. Hashemi Amrei - University of California, Davis

Dr. Scott Bukosky - University of California, Davis

Prof. Greg Miller - University of California, Davis

Prof. William Ristenpart - University of California, Davis

Abstract

We demonstrate that application of an oscillatory electric field to a liquid generates a long-range steady field, provided the ions present have unequal mobilities. The main physics is illustrated by a two-ion harmonic oscillator, yielding an asymmetric rectified electric field (AREF) whose time average scales as the square of the applied field strength. Computations of the fully nonlinear electrokinetic model corroborate the two-ion model and further demonstrate that steady AREFs extend over large distances between two electrodes. Experimental measurements of the levitation height of micron-scale colloids versus applied frequency and potential accord with the numerical predictions. We illustrate how the heretofore unsuspected existence of a long-range steady field helps explain several long-standing mysteries regarding induced charge electrokinetic flows in oscillatory potentials.

On the scale dependence of flow structures and transport in electroconvection near ion-selective membranes

Authors

Prof. Ali Mani - Stanford University

Ms. Karen Wang - Stanford University

Abstract

Electroconvection (EC) is a hydrodynamic phenomenon that occurs when dissolved ions are driven from a fluid towards an ion-selective surface. EC is important because it significantly alleviates transport limitations by concentration polarization. However, the structures of the flows in EC, their quantitative implications in transport, and its dependence on key input parameters are not well understood. While experiments of EC are lacking due to their resolution limits, performing simulations in parameter regimes relevant to industrial applications is also challenging; the widerange of spatiotemporal scales present in EC calls for costly computations with extremely high resolutions. In this study, we present results from direct numerical simulations of canonical settings to investigate the dependence of EC vortex scales on the key input parameters. We find that in the chaotic regime, the range of flow scales depends strongly on the nominal Debye screening length and only weakly dependent on the driving potential. We demonstrate that while the largest vortices are controlled by the macroscopic geometry, the smallest vortices scale with Debye length to the power of 0.8. Normalization based on this power law leads to collapse of various statistics over a wide range of input parameters. In conjunction with these results, we present an investigation using proper orthogonal decomposition (POD) of the flow fields to assess the importance of different flow scales in enhancing transport in EC. We show that a reduced representation using selected large-scale POD modes can capture the dominant transport. We further discuss implications of these results in strategies for reduced-order modeling of electroconvective flows.

Theory of electrokinetic transport in deformable nanochannels

Authors

Mr. Mpumelelo Matse - Simon Fraser University

Prof. Peter Berg - University of Alberta

Prof. Michael Eikerling - Simon Fraser University

Abstract

Electrokinetic transport phenomena, predominantly realized in charged polymeric and porous media, offer possibilities for applications in nanofluidic systems, energy harvesting and biosensing. In this work, we present a theoretical and numerical study of nonlinear coupling between wall deformation and the flows of water and ions in a charged, deformable nanochannel. The classical treatment of mass and momentum conservation in the solid-liquid coupled system is based on the Stokes-Poisson-Nernst-Planck equations. For elastic but non-viscous walls in the limit of small deformation, analytically solvable differential equations were obtained in one dimension. The response of the walls' relaxation dynamics and the channel's electrokinetic transport was investigated at different charging regimes. Within the framework of nonequilibrium thermodynamics, compact formulae in terms of Onsager's phenomenological coefficients were derived for the electrokinetic transport parameters and energy conversion efficiency. Furthermore, an extension of the model is presented for electroactuator modelling which operates through a coupling of electrical and mechanical interactions for closed nanochannels. In this scenario, we explore numerically the transient dynamics and steady-state solutions for closed, finite nanopores. A full theoretical account, along with numerical results, of the effect of membrane charging and mechanical response on the differential capacitance is presented.

The kinetics of jet impingement-induced HeLa cell detachment from graphene and graphene oxide

Authors

Prof. Lubomir Lapcik - Palacky University Olomouc

Mr. Jakub Vlcek - Palacky University Olomouc

Dr. Barbora Lapcikova - Palacky University Olomouc

Prof. Michal Otyepka - Palacky University Olomouc

Abstract

A broader and quantitative understanding of cell adhesion to two-dimensional carbon-based materials is needed to expand the applications of graphene and graphene oxide (GO) in tissue engineering, prosthetics, biosensing, detection of circulating cancer cells, and (photo)thermal therapy. We therefore studied the detachment kinetics of human cancer cells (HeLa) adhered on graphene, graphene oxide (GO), and glass substrates using stagnation point flow on an impinging jet

apparatus. HeLa cells detached easily from graphene at a force of 9.4 nN but adhered very strongly to GO. The presence of hydrophilic functional groups thus apparently enhanced the HeLa cells' adherence to the GO surface. On graphene, smaller HeLa cells adhered more strongly and detached later than cells with larger projected areas, but the opposite behavior was observed on GO. These findings reveal GO to be a suitable platform for detecting cells or establishing contacts, e.g. between graphene-based circuits/electrodes and tissues.

Particle rotation driven systems

Authors

Prof. Andrejs Cebers - University of Latvia

Abstract

Ensembles of externally driven rotating particles constitute a benchmark case of active systems. Particle rotation may be caused by different mechanisms, for

instance, by a rotating field in magnetic suspensions, whereas in a weakly conducting liquid subjected to an electric field particle rotation arises due to the Quincke effect. Here we analyze some general issues related to phenomena caused by particle rotations. One of them is the description of macroscopic flows in the frame of hydrodynamics with spin. The action of antisymmetric stress on the free boundary causes Couette like flow of the liquid, which may be regarded as the negative viscosity effect [1]. It should be remarked that a liquid flow may arise at electric field strength beyond the critical value at which spontaneous rotation of a single particle arises. It is illustrated that in the range of the electric field strengths close to the critical value shear banding may be observed. Interesting phenomena are observed in the case of the non-conducting particle covered droplets in the electrical field, when the particles are forming belts on the equator of oblate droplets [2]. By analysis of the instability of the belts in the frame of a Brinkman-like approximation it is illustrated that the belt is unstable against long wavelength perturbations.

In the case when lubrication forces between the particles are strong, the dynamics of ensembles of rotating cohesive particles are quite unusual. It is analyzed for ensembles of a limited number of particles and it is found that when the angular velocity of the particles is small the ensemble rotates as a solid body. At higher angular velocities stick-slip motion of the external layers with respect to the internal layers arises. These effects are rationalized in the frame of a Frenkel-Kontorova type model where the internal layer of the particles plays the role of the substrate. By numerical simulations it is found that stick-slip motion occurs by synchronized pairs of particles. Characteristic square root dependence of the average slip velocity on the driving force is obtained.

[1] A.Cebers, *Magnetohydrodynamics*, 16,175 (1980)

[2] M.Ouriemi, P.M.Vlahovska, *J.Fluid Mech.*, 751, 106 (2014)

Active Control of Viscous Fingering Using Electric Fields

Authors

Dr. Tao Gao - MIT

Dr. Mohammad Mirzadeh - Massachusetts Institute of Technology

Prof. Martin Bazant - MIT

Abstract

Viscous fingering is a widely observed phenomena in nature and many industrial processes in which finger-like instabilities occur at the interface of two fluids when a less viscous phase displaces a more viscous phase. Once the viscosities of these two fluids are given, there remains very limited freedom for controlling the interfacial stability. Here we show the interfacial stability of two immiscible electrolytes can be controlled, either suppressing or promoting finger growth, by applying an electric field parallel to the flow to couple electroosmotic flow to the system. Such an external field enables robust and easy control of the interfacial stability for any pair of fluids. Specifically, we demonstrate that a hydrodynamically stable displacement can be destabilized by applying electric field in the opposite of flow direction, and a hydrodynamically unstable displacement can be stabilized by applying electric field in the flow direction. Potential applications of this new discovery including increasing mixing efficiency of fluids by destabilizing interface and enhancing secondary oil recovery by stabilizing interface.

Electrokinetic Control of Viscous Fingering

Dr. Mohammad Mirzadeh - MIT

Dr. Tao Gao - MIT

Prof. Martin Bazant - MIT

Abstract

Pattern formation is ubiquitous in many physical and chemical processes. In many instances, interfacial instabilities play a central role in creating and controlling the patterns. Perhaps one of the most well-known examples is the “viscous fingering” instability which occurs a higher viscosity fluid is displaced by a lower viscosity one. This phenomenon was originally described by Saffman and Taylor for quasi two-dimensional flows in Hele-Shaw cells. Similar patterns naturally occur during two-phase flows in porous media where it leads to

residual trapping during secondary oil recovery and reduces extraction efficiency.

In the classical theory, the onset of instability is controlled by a single parameter, i.e. the viscosity ratio. However, coupling with other physiochemical processes could enhance or suppress viscous fingering. Here, we use linear stability theory as well as nonlinear numerical simulations to study the role of electrokinetic coupling on the interface stability. Our results indicate that viscous fingering may be controlled, and even suppressed, by applying external electric fields.

Ion Transport and Current Rectification in Nanopores Subject to Dual pH-Gradient and Voltage Bias

Authors

Ms. Tsai-Wei Lin - Department of Chemical Engineering, National Taiwan University

Prof. Jyh-Ping Hsu - Department of Chemical Engineering, National Taiwan University

Dr. Chih-Yuan Lin - Department of Chemical Engineering, National Taiwan University

Prof. SHIOJENN TSENG - Department of Mathematics, Tamkang University

Abstract

Modern advanced fabrication techniques make it possible to simulate the behaviors of biological ion channels through artificial nanopores/nanochannels, which are also widely adopted to regulate the transport of ions, thereby facilitating potential applications in areas such as ion pumps, energy conversion, ion gates, metal ion sensing, and bio-sensors. To realize these applications, a thorough understanding of the phenomena and the underlying mechanisms associated with the ion transport in a micro-/nano-scaled space, which are not present in larger scaled systems, is both necessary and inevitable. These phenomena include, for example, ion selectivity and ion current rectification. The latter arises mainly from an asymmetric ion distribution inside a

nanopore/nanochannel when a potential bias is applied. The transport of ions in biomimetic nanopores surface modified by polyelectrolytes was studied extensively in the last decade. The associated behavior can be influenced by factors such as the geometry and the charged conditions of a nanopore, the type and the concentration of salt in the liquid phase, and the solution pH. The last factor was studied theoretically by many investigators. However, most of them assumed a uniform pH profile across a nanopore. Although several experimental studies considered a non-uniform pH profile through applying an extra pH gradient across a nanopore, there is a lack of a comprehensive theoretical study.

It is known that applying simultaneously an electric potential and a pH gradient can improve appreciably the performance of the ion current rectification of a nanopore. Unfortunately, the underlying mechanisms are still not well understood. Adopting a cylindrical nanopore functionalized with homogeneous (single) pH-tunable polyelectrolyte brushes, these mechanisms are discussed in this study. In particular, the roles that the applied pH and electric potential gradients and the grafting density of the polyelectrolyte chains played are examined in detail. We show that homogeneously modified nanopores can also exhibit ion current rectification behavior that is only seen in nanopores functionalized with two or more kinds of polyelectrolyte. Several interesting results are also observed. For example, if the applied pH gradient is sufficiently strong, the preferential direction of the ionic current can be tuned by the level of the applied electric potential; if it is sufficiently weak, an increase in the grafting density of the polyelectrolyte chains can make that preferential direction reversed. These results provide not only explanation for the behaviors associated with the transport of ions in nanopores but also reference for designing relevant devices.

The Role of Thermal Voltage in Biology

Authors

Prof. James Sterling - Keck Graduate Institute

Abstract

Crowded macromolecular environments establish electrical potential gradients that result in transport of charged molecules by both diffusion and electrophoresis. In biological tissues, the motion is often dominated by electrophoresis even in the presence of naturally-established, seemingly small electric fields. The reason is that polymer reptation during electrophoresis in complex matrices leads to an electrophoretic mobility that is much larger than translational diffusion. In a reptation-regime of gel electrophoresis, electrophoretic mobility scales with the inverse of the length of the molecule while the diffusion coefficient scales with the inverse of the length to the 1.5 or greater power. The ratio of diffusivity to electrophoretic mobility for species i , known as the thermal voltage V_{Ti} , would therefore be expected to scale with the inverse of the square root of the molecular length.

In the absence of active transport due to pumps, channels, or facilitated transport, the spatial distribution of a species reaches quasi-equilibrium when diffusion and electrophoresis are balanced. The result is that charged species are partitioned according to

$$c_i(\mathbf{r}) = c_{io} \exp[-V/V_{Ti}]$$

where c_{io} is the concentration of the species in a location of zero potential. At the cellular level, biological potentials can vary by 10's to well over 100 millivolts with well-known values of cytosol potential in the range of -80 or -90 mV relative to the extracellular space and mitochondria interior between -100 to -180 mV, for example. Thus, ions at body temperature with $V_{Ti} = 26.7$ mV may partition between tissues in concentration ratios of greater than a factor of 50 to over 100, in the absence of ATP. Using experimental and theoretical polymer models, the thermal voltage of short single-stranded DNA oligonucleotides is found to be around 5 mV in free solution, 5kb DNA is near 0.1 mV and 10kb DNA is near 0.05 mV in agarose gels of concentration around 0.8 percent, for example. The result is that charged macromolecules may partition due to electrophoresis, even in tissues with small electric fields.

A mathematical model of biological tissues is presented that is based on reaction-electrophoresis mechanisms that include such macromolecular

transport. Focus is on reactions to represent Eigen-Tamm ion-pairing that includes contact ion pairing and solvent-separated ion-pairing and Poisson Nernst Planck (PNP) models for ions and multivalent biological molecules. The framework addresses how to characterize the interplay of electrophoresis and reaction of charged molecules in crowded macromolecular environments. Nucleic acids, glycans, and most proteins are anionic and are compensated by cation-specific binding and charge screening to achieve electroneutrality. In the context of this model, phosphorylation and sulfation mechanisms and the control of metabolic and secretory processes are discussed.

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Overlapping double layer effects on electrokinetic squeezing flow electrical power generation

Authors

Prof. Hsin-Fu Huang - Department of Mechanical Engineering, National Taiwan University

Mr. Shi-Wei Jian - Department of Mechanical Engineering, National Taiwan University

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Abstract

We study a novel electrokinetic streaming potential power generation method achieved by squeezing continuous phase liquid flows in parallel plate channel geometries with hydrophobic slippery wall boundaries. The key features relevant to this electrokinetic energy conversion arrangement are the reducing separation distance between the parallel plates and the electrical double layers respectively emanating from the upper and lower channel walls approaching one another over the duration of squeezing flow. However, linear non-overlapping double layer potentials were assumed in previous literature, and the non-linear aspects of overlapping electrical double layers as well as their influences on the performances of electrokinetic squeezing flow energy conversion are yet to be investigated. Distinguished from previous analyses, here we present a semi-analytical non-linear analysis on electrokinetic squeezing flow power generation of an arbitrary number of squeezing slit channels connected in parallel with an output load resistance in the regime of considerable double layer overlap. While the squeeze flow dynamical equations are solved in the unidirectional lubricating flow limit, we describe the double layer potential and spatial charge distributions within the parallel plate channel liquid space using the fully non-linear Poisson-Boltzmann equation and its subsequent Jacobian elliptic function solution. Two forcing modes, namely, the constant squeezing speed and constant squeezing force conditions, are considered, and the respective semi-analytical solutions to the instantaneous energy conversion efficiency, external load current, required force or resultant speed, streaming potential distribution, and power produced per unit force input are derived for the two modes and expressed in terms of the physical parameters relevant to the electrokinetic flow condition investigated herein. In addition, solutions and results obtained from the present non-linear analysis are further compared with those of a linear non-overlapping double layer analysis reported in previous literature so as to highlight the fundamental differences in the various aspects of electrokinetic squeezing flow energy conversion performance respectively due to the exact and approximated double layer

potentials. Parametric and comparative analyses show that for half channel height to Debye thickness ratios of one ($kh=1$), the linear non-overlapping double layer analysis underestimates the peak energy conversion efficiency as compared to the present overlapping double layer analysis. Moreover, the amount of underestimation in peak efficiency is generally reduced as the boundary slip length is increased to 100 nm. Over the duration of squeezing strokes from $kh=20$ to 0.5, the maximum attainable load current, (required) squeezing force, and streaming potential value are underestimated by the linear non-overlapping double layer analysis for the constant squeezing speed mode, whereas the non-overlapping analysis overestimates the maximum load current, resultant squeezing speed, and streaming potential value for the constant squeezing force mode. These results indicate that the energy conversion performances obtained from previous literature substantially deviate from those of the present investigation, and suggest that the non-linear aspects of overlapping electrical double layers are crucial to the theoretical modeling, practical design, and optimal operation of electrokinetic squeezing flow power generation which may potentially be applied in the development of portable or wearable micro-batteries and charging devices.

2D Patterned Ion-Exchange Membranes Induce Electroconvection

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Abstract

In this work, we exploit the positive zeta potential and the combination of micro and macro structure of P2VP-microgel patches on cation-exchange membranes for early and effective boundary layer mixing by electroconvective vortices.

All membrane based separation processes suffer from concentration polarization during operation. This effect is also prominent in electrodialysis, where ion-exchange membranes are used to separate ions in an electrical field. The resistance of the system notably rises when the process is operated above the so-called limiting current density due to the depletion of ions in the laminar boundary layer. Here, the ion transport towards the membrane is diffusion-limited. This manifests in a plateau, where the current stagnates even though the driving force is increased.

In contrast to non-electrically driven membrane processes, a further increase in driving force leads to a third regime of increasing current. At sufficient high applied potential, electroconvective vortices occur mixing the boundary layer.

Thereby, solution of high concentration is transported from the bulk to the membrane.

Much work in literature is dedicated to investigate the influence of membrane surface properties on the introduction of electroconvective vortices. Early appearance of vortices shortens the plateau length by providing efficient mass transfer through the boundary layer. We found a promising procedure for early and strong vortex evolution. Experiments showed that membranes modified with P2VP-microgel patterns by inkjet printing do exhibit a significantly decreased plateau length at a simultaneous increased voltage until depletion occurs [1].

We suppose that the surface charge of the patterns has a big impact on the evolution of electroconvection and on the ion transport close to and above the limiting current, as also indicated in literature [2]. Therefore, the influence of charged patches is investigated in 2D computational fluid dynamic simulations to further understand and exploit this phenomenon. The simulations indicate that the surface charge of the printed patterns influences the initial direction of the vortices. Such vortices transport solution of high concentration from the bulk above the patterns to uncovered areas between patches. This way, hydrodynamics support the desired migration. In contrast to that, patches bearing a negative surface charge build up a reversed hydrodynamic transport. Bulk solution is transported from the uncovered area to the area above the patches. The field-induced migration is opposed to the vortex direction.

Further simulative and experimental investigation is ongoing. Additional knowledge of the significant phenomena for early and effective electroconvection enables tailor-made membrane surfaces to minimize ion depletion.

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Parallelized Electrorotation in single cell DEP micro cages

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Abstract

Electrorotation analyzes cells in suspension by placing them in rotating electric fields. The cells polarize and start rotating too. Their speed of rotation depends on the resonance of the polarization based on their inherent dielectric properties and the frequency of the rotating electric field. Observing the speed of rotation reveals their dielectric properties. This technique is especially powerful to investigate the membrane properties of cells. Electrorotation has been used to investigate the dielectric properties of cells in suspension within fluidic chambers of multiple hundred micrometers of diameter. Many cells have been pipetted into the chamber and their mechanical response to the electric field actuator was observed. Later, electrodes for electrorotation were integrated in microfluidic channels, which enabled to investigate cells subsequently one by one. However, the amount of cells is limited due to the rather long analysis duration of electrorotation and the fact that cells are not investigated in parallel.

Our laboratory recently developed a technology to fabricate 3D electrodes by sputtering conformal metal on a SU-8 skeleton followed by mask less ion beam etching. The directional etching process attacking the top of the wafer removes the metal on the planar surfaces, but leaves the metal on the side walls of the SU-8. Using this technique, we could fabricate two array of free standing 3D electrodes across a wide microfluidic channel. Each electrode is individually addressable by wires integrated in the ground of the microfluidic channel.

With no electric signal applied, cells driven by the flow simply traverse the electrode arrays. Applying an 100 kHz signal of ± 1 V at the upstream and ± 5 V at the downstream electrodes, a small dielectrophoretic entrance and a larger dielectrophoretic exit barrier is created. Cells can overcome the first entrance barrier but not the second exit barrier and are consequently trapped in the array. Individually increasing the electric signal at the entrance electrodes of a micro cage, where a cell was trapped, from ± 1 V to ± 5 V prevents additional cells to enter the trap. After a sufficient number of cells is trapped all micro cages are closed by increasing the applied voltage and the DEP trapping signal is alternated with an electrorotation signal (phase shift of 90° between neighboring electrodes). The electrorotation spectra of the cells are acquired by observing the cells under the microscope and reading out their speed of rotation with a pattern matching algorithm, while sweeping the frequency of the rotation signal. Removing selectively the electric signal at the exit electrodes can individually release the cells after the measurements.

Using this platform, we could for the first time acquire the electrorotation spectra of multiple single cells in individual micro cages in parallel. This sets the basis in order to upscale electrorotation for rare cell research applications. Following the experimental procedure describe above, we could reveal the dielectric properties in agreement with the literature for human immortalized T lymphocytes, HeLa and HEK 293 cells. Additionally, we could investigate the specific membrane capacitance of M17 neuroblastoma for the first time.

Electrokinetic Ion Transport in an Asymmetric Double-gated Nanochannel

Authors

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Abstract

Bioinspired, nanoscale artificial functional nanochannels for intelligent molecular and ionic transport control have versatile potential applications in nanofluidics, energy conversion, and drug controlled release. To simulate the gating and rectification functions of biological ion channels, we model the electrokinetic ion transport phenomenon in an asymmetric double-gated nanochannel having a pH-regulated, zwitterionic surface. Taking account of the effect of electroosmotic flow (EOF), the conductance of the nanochannel and its ion current rectification (ICR) behavior are investigated and the associated mechanisms interpreted. In particular, the influences of the solution pH, the bulk salt concentration, and the base opening radii and the surface curvature of the nanochannel on these behaviors are examined. We show that through adjusting the base opening radius and the surface curvature of a nanochannel, its ICR behavior can be tuned effectively. In addition to proposing underlying mechanisms for the phenomena observed, the results gathered in this study also provide necessary information for designing relevant devices.

Electrokinetic enhancement of ion transport through changing membrane topology

Authors

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Abstract

Fundamental understanding of ion transport processes in electrodialysis (ED) processes is of importance to enhance efficiency in these systems. In typical ED processes a potential is applied over a stack of alternating cation- and anion exchange membranes, yielding alternating compartments enriched and depleted in the electrolyte. ED can only be industrially operated at relatively mild potentials, as above a critical voltage no additional ions are transported as a result of diffusion limitations in the feed solution ("limiting current"). However, at the so-called "overlimiting current", increased ion transport is observed. Electrokinetic flows induced by local concentration and electric field gradients are considered to be one of the mechanisms leading to this overlimiting current. Here, we investigate the effect of membrane and microchannel geometries on the development of electrokinetic transport of ions.

We experimentally investigate electrokinetic flows adjacent to charge selective interfaces using a microfluidic ED-platform [1] consisting of alternating rows of positively and negatively charged hydrogels. The charge selective hydrogels can be patterned in PDMS chips allowing for access to different geometries and providing a platform for rapid investigation of topological effects. This approach is motivated by theoretical work relating to geometric patterning of membranes and spacer topologies to enhance ion-transport. Our experimental platform provides an excellent model system to investigate the influence of such geometric patterns as it allows for direct visualization of depletion/enrichment behavior simultaneous with electrical characterization.

Experiments were conducted using salt solutions of different concentrations seeded with charged fluorescent dyes to visualize local ion concentration. By means of fluorescence microscopy using a negatively charged dye we visualized the formation of depletion zones near different hydrogels, both with and without cross flow. In order to quantify concentration profiles in the system, we used Fluorescence Lifetime Image Microscopy (FLIM) to measure local chloride ion concentrations near the hydrogels and compare these to the fluorescence

microscopy results. Numerical simulations of the electric field distribution through the different geometries were done for the

For different geometries, we find that the development of these depletion zones is distinctly different as a result of the distribution of the electric field lines through the different geometries. Pinning of depletion zones occurs in heterogeneously patterned systems, and enhancement in the total transport is observed with increasing system heterogeneity as a result of electroosmotic contributions to the charge transport towards the selective interface [2]. Tangential components of the electric field are induced as a result of the geometric features of the system, yielding increased ion transport in all characteristic regimes, from Ohmic to overlimiting. Electrokinetic instabilities at the interface are observed at elevated potentials, increasing the total current through the hydrogels. This indicates that electroosmotic and electrokinetic contributions to the total charge transport can be enhanced by inducing non-uniform electric fields using membrane topology variations and spacers.

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Chemically modified activated carbon for high performance capacitive deionization

Authors

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Abstract

Capacitive deionization (CDI) is electrochemical process which considered as a promising alternative to established water desalination technologies. This new growing CDI technology need to overcome the following: 1. low performance electrodes 2. short lifetime 3. low energy and cost-effectiveness. The efficiency and kinetics of the continuous salt removal process via CDI can be improved significantly by optimizing electrodes without using less common or highly elaborate novel materials. In this study, we attempted to synthesize high performance electrodes in which double layers are obtained by applied potential

and adsorption of selective ion by ion-exchange process; the activated carbon was functionalized with charged functional groups (i.e. positive charge & negative charge), this leads to the spontaneous attraction to the selective charge only at ion-sorption step. The noble carbon electrodes exhibit enhanced (2x) salt adsorption capacity while also possibly decrease the overall cost of the MCDI cell. The experimental results on this study will be presented in detail.

Theory of ion and water transport in electron-conducting membrane pores with pH-dependent chemical charge

Authors

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Abstract

In this work, we develop an extended uniform potential (UP) model for a membrane nanopore by including two different charging mechanisms of the pore walls, namely by electronic charge and by chemical charge. These two charging mechanisms will generally occur in polymeric membranes with conducting agents, or membranes made of conducting materials like carbon nanotubes with surface ionizable groups. The electronic charge redistributes along the pore in response to the gradient of electric potential in the pore, while the chemical charge depends on the local pH via a Langmuir-type isotherm. The extended UP model shows good agreement with experimental data for membrane potential measured at zero current condition. When both types of charge are present, the ratio of the electronic charge to the chemical charge can be characterized by the dimensionless number of surface groups and the dimensionless capacitance of the dielectric Stern layer. The performance of the membrane pore in converting osmotic energy from concentration difference into electrical power can be improved by tuning the electronic charge density on the pore.

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Thermodynamics of soil electrokinetic treatment

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Abstract

Due to the amount of polluted sites reported as environmental emergencies and its toxic effect on the surrounding population a solution it's necessary. One of the many possibilities it's to apply an electro-kinetic treatment, which is a non-destructive in-situ process. During an electro kinetic treatment the main transport phenomena are: Electro-osmosis, electro-migration and electrophoresis, this phenomenon removes the species that are already present in the soil solution. However they are also adsorbing species in the wet soil, which need to be desorbed so they can be removed by electro-kinetic transport phenomenon. The study of the adsorption/desorption process that occur at the

soil-pollutant-soil solution interphase allow to analyze the chemicals conditions that will generate desorption of pollutant species. The ζ it's the parameter that interconnects the physicochemical properties of the soil-pollutant-soil solution interphase, and the ζ values reflect desorption/adsorption process that occurs in this interphase. This study is done prior to the electrokinetic tests, the ζ measurements reduce the generation of waste and you will not need testing electrokinetic with different electrolyte solutions in cell, it will be only necessary to perform test with the solution that cause greater desorption, solubility and mobility of the species. In this work the ζ values are used to describe the mobility of species through the soil sections in a work cell (Osmic -I) by applying an electrokinetic treatment. The samples used for this study are two model soils kaolin (C) and bentonite (B), also a sample from the mining waste of Zimapan (Z), Hidalgo. First the soil-cation interaction was analyzed with the preparation of homoionic samples of B and C soils, with the exchange of the surface H^+ by Na^+ , Cu^{2+} and NH_4^+ , to compare the adsorption selectivity of metal species on the soil surface different cations were exchanged in the form of sulphates and chlorides salts. The adsorption/desorption process at the soil-cation interface finally obey the law of chemical equilibrium, so the tendency of these processes depends not only on the electrical and electrochemical properties (surface charge density, hydrated ionic radius, coefficient transport, ion mobility), but also depend on the chemical affinity of the species present at this interface by which the analysis should be considered chemical properties. Pollutant species must be in the soil solution to be removed by electrokinetic transport phenomena, which is why the study should focus primarily on the effect of the electrical and chemical affinity of the cation. The selection of the electrolytic solution must fulfill the conditions that cause desorption of these species, thereby removing the pollutants depend on the intensity of the soil-cation interaction. The results indicated that the used of ammonium citrate solution is the one that generated more desorption in the three soil samples. The soil-cation interaction is reflected on the z value measured, the adsorption energy is calculated by the proposed equation and present a tendency related with the specific adsorption of cations described by the Hofmeister series. Also the effect of the ion pair is reflected on the adsorption process.

Electrokinetic Scanning Probe for Localized Surface Patterning and Analysis

Authors

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Abstract

We present a theoretical analysis and experimental demonstration of a new concept for a non-contact scanning probe driven entirely by electric fields, able to locally interact with confined reaction sites on biological and chemical interfaces in liquid environments. We demonstrate that the electrokinetic scanning probe (ESP) can accurately control the size of the confinement and reaction conditions, and can be used for wet-in-wet printing, suitable for various biological applications.

The device consists of a microfluidic chip having two reservoirs connected via narrow microfluidic channels leading to the chip's apex. The chip is dipped vertically into an immersion liquid and is positioned at a ~ 10 μm -scale distance from a surface. By injecting a sample through one channel and aspirating it through the other, a localized flow confinement is obtained. The ESP is based on electroosmotic aspiration, where an electric field is applied between an electrode in the aspiration reservoir and two ground electrodes at the apex, located symmetrically relative to the apertures, thus establishing electroosmotic flow. Utilizing a low ionic strength buffer as immersion liquid guarantees significant EOF in the aspiration channel, allowing to use high ionic strength processing solutions compatible with biological applications. Since the injected sample composition may vary, we use gravity as our primary injection

mechanism, with flow rate dictated by the hydrodynamic resistance of the injection channel. The injection channel can be augmented with its own electric field enabling to further increase the flow rate of the injected sample. The size of the confinement can then be accurately controlled by adjusting the ratio of the electric fields applied across each channel.

The electrokinetic actuation enables generation of stable, fluctuation and bubble-free flow confinements, which consume low volumes of samples, with essentially no dead volumes. Owing to its non-contact operation, the ESP can scan multiple reaction sites in a short time. We demonstrate an accurate control of the size of the confinement area, compatibility of the ESP with a wide range of processing solutions, pH range, and its applicability for patterning of DNA on glass and nitrocellulose surfaces, local heating of surface-based samples, and melting curve measurements.

The ability to electrically drive the confinement of liquids in the “open space” provides a new level of fluidic control, and opens the door to a range of new applications in deposition and extraction of molecules to- and from- a variety of surfaces.

Electrorotation of semiconducting microspheres

Authors

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Abstract

We have synthesized semiconducting (ZnO) particles and measured their electrorotation spectra in KCl aqueous solutions. Experiments show that two distinct particle populations are present in our samples: (A) smooth microspheres that rotate counterfield for frequencies of the electric field around hundreds of kHz; and (B) rough quasi-spherical particles that also rotate

counterfield at frequencies slightly smaller and, additionally, they show co-field rotation for frequencies higher than 1 MHz.

We compare experimental data with a recent theoretical analysis of the electrokinetics of semiconducting spheres [1]. The behavior of the rough spheres (B) is in agreement with a theoretical model that accounts for the charging of the electrical double layer at the particle-electrolyte interface. On the other hand, the results for smooth spheres (A) are described by a shell model that consists in a dielectric layer surrounding a lossy-dielectric medium. We use electron microscope techniques (SEM, TEM and EBSD) to investigate the internal structure of these spheres and find that spheres B are homogeneous particles with crystalline structure at large scales, while spheres A show a concentric stratification and a low crystallinity.

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AC electrokinetics in a deterministic-lateral-displacement device

Authors

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Abstract

We study the different forces that play a role in the separation of particles in a deterministic-lateral-displacement (DLD) device actuated with electrokinetic forces. A DLD device consists of an array of posts placed in a microfluidic channel. The array of post presents a certain tilt angle to the fluid flow so that left-right symmetry is broken in the microchannel. Particles in suspension are separated based on size when the suspension flows through this channel with posts: particles with a diameter greater than a critical diameter are diverted,

while particles smaller do not change direction. Here, AC electric fields are applied to the DLD device in order to improve particle separation and produce a tunable device. The AC electric fields are applied perpendicularly to the flow direction by planar electrodes placed at both sides of the channel. Experiments show that at low frequencies (up to 500 Hz) particles oscillate in the direction of the field due to Electrophoretic (EP) and/or Electroosmotic (EO) forces while they are dragged by the flow. As the frequency of the field increases beyond 1 kHz, the amplitude of these oscillations becomes negligible and, eventually, dielectrophoresis (DEP) becomes the dominant electrokinetic force on the particles. Dielectrophoresis arises from the electric field inhomogeneities caused by the presence of the DLD dielectric posts. These mechanisms alter the particle path inside the DLD devices leading to separation of particles depending on electrokinetic properties. It is shown that the AC electrokinetic forces are able to divert particles with diameters smaller than the critical in the absence of electric fields, so that enhancement of sorting is achieved [1]. We analyse the forces that lead to particle diversion depending on the frequency of the applied voltage. At high frequencies, particles are diverted by negative dielectrophoresis. At low frequencies, we propose that particles, in their oscillating path, interact with the posts in a way akin to wall-induced lateral migration in particle electrophoresis [2].

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Dielectrophoretic-driven deformations of a lubricated elastic sheet

Authors

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Abstract

The ability to deform an elastic interface into a desired pattern has potential use in a wide range of applications, such as reconfigurable lab-on-a-chip devices, soft robotics and adaptive optics. One promising approach to induce such deformations is to utilize dielectrophoretic (DEP) forces that act on elastic dielectric materials due to the presence of a non-uniform electric field. However, up to date, the use of DEP forces has been primarily investigated in the context of manipulating discrete objects, particularly particles and cells. In this work, we present a theoretical model and experimental demonstration for the deformations of an elastic sheet suspended on a thin liquid layer due to an electric field established by a set of interdigitated electrodes. We provide an analytical expression for the electric field in a 3-layer configuration consisting of the liquid, elastic sheet, and air. Using the electric field, we analytically compute the force distribution on the sheet through Maxwell's stresses. Coupling this force with viscous flow and elastic deformation in limits of small deformation and negligible inertial effects, we obtain an analytical solution for the deformation of the sheet in time. We use this expression to study the effects of permittivity, conductivity, electrode geometry, and frequency on the resulting deformation. We use digital holographic microscopy for real-time monitoring of deformations induced by an interdigitated electrode array covered by a film of oil, demonstrating the phenomenon and enabling characterization of the deformations in support of the theoretical model.

Modelling of field-induced orientation and impedance in suspensions of conductive and insulating ellipsoids: Is the orientation determined by the principle of maximum entropy production?

Authors

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Abstract

For ellipsoidal objects, the impedance of suspensions can be described by analytical equations derived with the mixing equation of Maxwell and Wagner. The impedance depends on the objects' axis ratio and orientation. For axisymmetric ellipsoidal objects (spheroids), with their symmetry axes being oriented in parallel, in perpendicular or at random with respect to the external field, the results can be simplified further by combining them with the influential radius approach [Gimsa & Gimsa. J. Electrostatics 90 (2017) 131–138 doi:10.1016/j.elstat.2017.10.0082]. The approach also makes it possible to derive the torques induced by the external AC field at the objects. As has been demonstrated in experiments with triaxial chicken erythrocytes, the torques tend to orient the axes with the highest real part of the Clausius-Mossotti factors in the field direction. For the limiting cases of conductive or insulating spheroids, these are the longest axes of the objects. Conductive and insulating disks will be oriented with their symmetry axes perpendicular to the field, whereas conductive and insulating needles will be oriented with their symmetry axes in parallel to the field.

Considerations show that the field-induced orientations lead to a reduction of the impedance of the suspension, a current increase and thus to an increased dissipation of electrical energy. Although the torque approach is based on electrostatic assumptions and neglects dissipation, it can probably explain object orientations more successfully than the well-known approach, which assumes that orientation minimizes the free energy of the suspension system.

It assumes the equivalence of a minimization of the energy and the field-induced torque acting on the individual objects. Nevertheless, it is believed that the free energy criterion is generally not appropriate for dissipative systems. The success of the torque approach in explaining the experimental results and its equivalence with minimizing the impedance of the suspension suggests a possible third approach that has not yet been used. This new approach takes entropy production into account.

At constant field, the entropy production, i.e., the dissipation of electric energy, is inversely proportional to the suspension's impedance. Under the assumption that the suspension system is near equilibrium in its linear range, entropy production should be minimized by object orientation according to Prigogine's principle. Nevertheless, there are at least two arguments that contradict this assumption: i) nonlinearity is introduced because the field-induced orientation changes the suspension's impedance; and ii) the experimentally proven torque criterion leads to a reduction of the suspension's impedance. Obviously, field-induced orientations follow the maximum entropy-production principle rather than Prigogine's principle. The law of maximum entropy production was formulated by Swenson 1989: a system will select the path or assemblage of paths out of the available paths that minimizes the (electric) potential or maximizes the entropy at the fastest rate, given the constraints. An elaborate discussion of the thermodynamic aspects of the three approaches is still required. The derived simplified equations may be helpful for gaining insights into new aspects of the interrelation of the impedance of suspensions with electrokinetic force and torque effects acting on suspended ellipsoidal objects.

Do We Need to Pose a Closure Problem to Capture the Dynamics of the Capacitive Charging of Porous Electrodes?

Authors

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Abstract

Porous conductive electrodes are often used in electrochemical systems to drive transport processes via electrochemical reactions or capacitive charging. Typical electrodes are carbon-based and upon charging develop electric double layers (EDLs) along pore. Electrodes undergoing capacitive charging, without electrochemical reactions, are used for several applications, such as supercapacitors where the EDLs are exploited for energy storage¹, and capacitive deionization (CDI) where the formation of EDLs in aqueous solutions is used for water treatment².

Such porous electrodes often possess a complex and spatially random internal pore structure. In order to model transport processes in such structures, often volume averaging is employed, a technique mathematically similar to Reynold's averaging in turbulent flow models. One important characteristic of the turbulent flow problem is that the non-linear advection terms of the Navier-Stokes equations results in the introduction of new variables upon Reynold's averaging and so lead to a closure problem. In electrochemical systems, transport equations contain nonlinear electromigration terms. However, the closure problem has been typically neglected *ad hoc*, for example by assuming "slowly varying variables"³, where the concentration and potential perturbation is assumed to be much smaller than the volume-averaged value. To our knowledge, only the work of Gabitto and Tsouris posed and solved the closure problem for capacitively charging porous electrodes⁴. Posing and solving the closure problem results in a more accurate solution at the cost of significant mathematical complexity.

We here study whether a closure problem is necessary towards accurately modeling transport processes in cells involving capacitive electrodes, neglecting surface transport phenomena⁵. As presented by Gabitto and Tsouris, the closure problem leads to a solution for tortuosity factor and local concentration and potential perturbations. In the current work, we present two constraints which are required to neglect the effect of perturbations. To investigate our findings, we developed a 2D local (in-pore) model capturing salt and charge dynamics during charging, and also volume-averaged the 2D model to obtain a 1D averaged model. We compared the results of the 2D local model and the 1D

model, with and without tortuosity term, for various pore geometries, including slit-shaped and with rough walls. This comparison leads to conclusions on whether it is important to pose and solve the closure problem in the capacitive charging of porous electrodes.

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AC electrokinetics of salt-free, multilayered soft particles

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Abstract

Interest in the electrical properties of the interface between soft nanoparticles and solutions is out of any doubt. Indeed, these particles are intended to be

used mainly in aqueous systems, where the electrostatic (and/or electrosteric) interactions dominate the system behavior and, very important, its response to external fields. Of particular significance is the case of **polyelectrolyte-coated particles**, mainly taking into account that the layer-by-layer procedure allows to control the thickness, permeability, and overall charge of the coated particle [1]. Like in simpler systems, electrokinetic determinations in ac fields (dielectric dispersion and dynamic electrophoresis by electroacoustic methods in the kHz to MHz frequency domain) provide the widest range of information about the physics of the interface: this includes the volume charge density of each layer, its thickness, the degree of interpenetration between layers or the overall size distribution of the coated particles. Different models exist on the electrokinetics of particles coated by a single layer [2,3], but studies regarding *multilayered particles* are certainly more scarce [4], and even more in the case of *salt-free* systems: ideally, the only charges existing in this case consist of the charge on the layers and the core particle itself, and their corresponding countercharges, with no other added ions, just those **released** by the particles upon charging. A salt-free suspension can form short- or long-ranged ordered phases with phase transitions at a relatively low volume fraction of particles. Due to the analogies with atomic or molecular crystals they are usually called *colloidal crystals or glasses*. In addition, their electrokinetic properties may resemble those of particles in non-aqueous media. In any case, the practical absence of ions other than those released produces electrokinetic responses far more complex than in salt-containing suspensions. A model will be presented for evaluating the dynamic mobility and the complex electrical conductivity (or complex dielectric permittivity) of these systems. The results will be used in order to explain experimental data obtained on both kinds of determinations using latex particles (500 nm in radius) coated with different polymer combinations (PDADMAC, PDADMAC/PSS, PDADMAC/PSS/PDADMAC) and without addition of further ions to the supporting solution.

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Theoretical analysis on the influence of viscous effects on the acoustophoretic trapping

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Abstract

From an analytic standpoint the solution for acoustic streaming phenomenon, generated by a standing acoustic wave (SAW), of a non-Newtonian fluid through a parallel flat plate microchannel is studied. An appropriate combination of the momentum equation together with the rheological Maxwell model, adopting the nondimensionalized version of the governing equations, allows us to obtain the following dimensionless parameters that control the fluid flow conditions: The Mach number ($M=A\omega/c_0$), the Deborah number ($De=\lambda_1\omega$), the ratio of the geometry of the channel ($\epsilon=H_0/L$), and the ratio between the height of the channel and the viscous boundary layer ($\alpha=H_0/d_{\nu}$). In the limit when $M \ll 1$ we obtain the hydrodynamics of the system using regular perturbation method. In the present work, we show that the acoustic trapping mechanism is controlled by the Deborah number and the ratio α . In channels that are width in comparison with the viscous penetration ($\alpha \gg 1$), corresponding to the Rayleigh streaming regime, the influence of the rheological characteristics can

be neglected. In channels having intermediate width ($100 > \alpha > 1$), the effect of viscoelastic model is notable.

Dielectrophoresis Based Characterization of LEA Proteins

Authors

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Abstract

Desiccation tolerance is unusual in eukaryotes, few organisms such as plants, lichens, algae, and invertebrates can withstand such abiotic stress; moreover, desiccation tolerance is mainly widespread among plant seeds which proved to survive for long period of time without water and are thus anhydrobiotes. Survival without water relies on an array of mechanisms designed to repair and protect the structure and the components of cells and tissues. A class of hydrophilic proteins expressed in late seed development, the so-called late embryogenesis abundant (LEA) proteins.

Understanding the mechanism of LEA protein can enhance engineering crops more tolerant to water stress and might be useful to develop new techniques to preserve cells and tissues in dried condition at room temperature which will be saving a lot of efforts and costs.

3DEP (DEPTech Ltd) platform was used to characterize the mechanism of different LEA proteins from the brine shrimp *Artemia franciscana* (a primitive arthropod that lives in saline water [1]) in the *Drosophila melanogaster* cell lines Kc167 (12-15 μm in diameter). Three different Kc167 cell lines were prepared to study their DEP measurements and spectra. (i) Kc167 cells are used as a control line, while (ii) Kc167 containing AfrLEA1.1, a group 1 LEA protein which resides in the cytoplasm with a total of 182 amino acids, as well as (iii) Kc167 containing

AfrLEA3m, a group 3 LEA protein which resides in the mitochondria with a total of 307 amino acids.

The Kc167 control cells and cells containing either AfrLEA1.1 or AfrLEA3m proteins were suspended in 50 $\mu\text{S}/\text{cm}$ conductive media with an osmolality of 0.38 osmol/kg (isotonic) and 1.8 million/ml cell concentration required to obtain reliable DEP spectra. Another media is prepared with an osmolality of 0.8 osmol/kg (hypertonic) where the 3 cell lines will be suspended for a stress study assessment. The DEP spectra of these three distinct cells are then analyzed in both cases to extract their dielectric properties to understand the mechanism and the effect of each LEA protein group on cells cytoplasm and membrane integrity when conferring stress.

Conclusion

DEP spectra of three different Kc167 cell lines were obtained, showing minor differences between the membrane properties of control line cells and cells containing any of the LEA proteins in isotonic media. However, at higher frequencies in the DEP spectra the cytoplasm properties of the cells were found to be significant, especially with the cells containing AfrLEA3m protein, indicating its activity is majored inside the cytoplasm more than in the membrane. Cells expressing LEA proteins showed preservation in membrane integrity when conferring stress (hypertonic media), while control cells' membrane were compromised due to the osmotic stress.

Electrohydrodynamic scaling laws analysis in a microfluidic isoDEP device

Authors

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Abstract

Dielectrophoresis (DEP) is the phenomenon in which a particle, such as a living cell, is moved by the interaction between a non-uniform electric field and its induced polarization. Isomotive dielectrophoresis (isoDEP) is a single cell analytical technique that uniquely applies a constant gradient field- squared () *resulting in a uniform DEP force. The resultant constant (isomotive) particle translational velocity can be tracked using particle tracking velocimetry (PTV) software to subsequently extract the cell/particle dielectric properties. This approach should significantly increase the throughput of acquiring a dielectric spectra of a single cell compared to electrorotation.*

DEP depends on polarizability of both the particles and suspending medium, the particles' size and shape, and the frequency of the electric field. However, DEP is not the only acting force on particles inside a microfluidic device; other forces include, but not limited to, drag force, gravity, A.C. electro-osmosis, electrolysis, buoyancy, and electrothermal forces (ETH). Hence, to enhance the DEP force over other forces several design parameters (e.g. microchannel width, height, base material, lid thickness, and AC voltage) must be tailored for each application or cell size. Because there are two ways of creating isoDEP (microelectrode and insulative) and there are many dimensions and material parameters to choose from, we are using a scaling law approach for future designs. For the same applied AC voltage, decreasing the height of the microchannel by 1/10th will decrease the velocity of ETH induced flow (V_{ETH}) by 100 times. Bonding a PDMS microchannel to a silicon base instead of a glass substrate results in 20x reduction in V_{ETH} . In this work, several fabrication and device designs have been made to obtain a better DEP analysis microfluidic device that was used to investigate the properties of phytoplankton cells. It was concluded that devices fabricated by full depth etching using DRIE to create the microchannel (microelectrode) resulted in a good DEP response at lower voltages compared to devices made from PDMS microchannel bonded to patterned ITO coated glass electrodes. However, rough wall surface containing etched silicon spikes generates high localized electric field that generates localized heating which in turns generates electrothermal vortices that compromises the operation of the device. Hence, isoDEP microchannel made from insulative PDMS insulative can minimize this ETH effect by making electrodes in far sites from the analyzing window. In addition, it can be easily

tailored to the desired cell size and microchannel height, but it requires a higher AC voltage amplitude which requires expensive amplifiers to provide high amplification at high frequency.

Insights into the Electrokinetic Effects on Oil Recovery at the Pore-Scale in Carbonate Rocks

Authors

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Abstract

Understanding the effect of injection water chemistry is becoming crucial, as it has been recently shown to have a major impact on oil recovery processes in carbonate formations. Various studies have come to the conclusion that surface charge alteration is the main mechanism behind the observed change of wettability towards water-wet due to SmartWater injection in carbonates. Therefore, understanding of the surface charges at brine/calcite and brine/crude oil interfaces becomes important to optimize the injection water compositions for enhanced oil recovery (EOR) in carbonate formations.

In this work, the physicochemical interactions of water, crude oil, and carbonates are analyzed using Surface Complexation Modeling approach (SCM). The zeta potential of brine/calcite and brine/crude oil interfaces are determined for different water ionic compositions. The SCM results are validated with

experimental zeta potential measurements of calcite/brine and crude oil in brine suspensions.

Then, a numerical model is built to study the effect of oil/brine and brine/carbonate zeta potentials on multiphase flow at the pore level. The flow dynamics is modeled by solving the hydrodynamic Navier-Stokes equations for an oil droplet mobilized by water inside a single pore. The effect of surface charges is taken into account through the DLVO (Derjaguin, Landau, Verwey, and Overbeek) theory of intermolecular forces, where experimental values of the zeta potential have been used in the model. The simulation results clearly show that the water ionic-composition has a strong impact on the pressure required to recover oil at the pore level. This strong effect of water chemistry indicates that waterflooding efficiency can be increased by optimizing the injected water salinity parameters for a given carbonate formation and crude oil properties.

Orientation effects in hydrodynamic instability in concentration polarization

Authors

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Abstract

One dimensional steady state passage of the electric current from an aqueous electrolyte solution into a charge selective (perm-selective) solid, such as a metal electrode or ion exchange membrane, is hydro-dynamically unstable. For a long time this instability has been attributed to electroconvection related to the extended space charge which forms at the outer edge of the electric double layer at the limiting current. For a perfectly perm-selective solid with infinite conductivity this mechanism is the only possible one. Recently, it has been shown that for a non-perfectly perm-selective membrane, or for a perfectly

perm-selective membrane with finite conductivity (commercial ion-exchange membranes are practically perfectly perm-selective), additional electroconvective instability mechanisms non-related to the extended space charge are possible, Phys. Rev. Lett. 114, 114502 (2015), Phys. Rev. Fluids 2, 093702 (2017).

All of the aforementioned studies focused on electro-convective instability mechanisms because it was recognized that the gravitational mechanism could not yield instability for most practical situations (sub-millimeter electrolyte systems with concentration below one centimolar and without a forced stirring). In such systems, the passage of electric current results in formation of concentration variations near the perm-selective solid known as concentration polarization (CP). The expression of CP is a characteristic voltage current dependence with a current saturation at the limiting value (limiting current, corresponding to a nearly vanishing interface electrolyte concentration) followed by a current increase with voltage known as the over-limiting conductance regime. For some systems, transition to the over-limiting conductance is accompanied by the appearance of excessive electric noise. Commonly, over-limiting conductance sets on due to the mechanical stirring of the interface diffusion layer resulting from hydrodynamic electroconvective instability of quiescent electric conduction. In relation to possible gravitational mechanisms, the CP-induced density stratification results both from direct concentration variation and its related non-uniform Joule heating. The temperature variations related to the latter usually do not exceed one degree Kelvin. As a result, for gravitationally unstable orientation with the depleted interface at the bottom, the Rayleigh number related to the thermally induced density stratification is usually smaller than that related to concentration variation, whereas the latter is lower than the Rayleigh-Benard instability threshold. For this reason, electro-convective mechanisms have been invoked to explain the instability, and no systematic study of the Joule heating effects in CP has been undertaken until recently (not long ago, the effect of density stratification related to concentration variation upon the electroconvective instability in CP has been addressed in

Phys. Rev. Lett. 116, 194501 (2016)).

Lately, this shortcoming has been remedied in the theoretical studies by Demekhin and his group, Phys. Rev. E91, 063006 (2015). They discovered a very interesting possibility of a Joule heating related instability expected to occur for overall stable density stratification (depleted interface on the top). In this presentation we investigate this possibility both experimentally and theoretically.

Mechanisms of ion transport in nanopores with conductive walls: new mathematical models and experimental results

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Abstract

In recent years, the studies of ion transport in nanopores and nanochannels have attracted increasing interest. They are of fundamental importance in various fields of science and technology, such as separation and purification of mixtures, electrochemical energy conversion, chemical sensors, and cell physiology. A modern and perspective direction is the development of 'smart' nanoporous membranes, which selectivity can be switched or tuned by external stimuli. A new class of membranes containing gold nanotubules in a porous polymeric support was suggested in [1]. It was shown that their selectivity can be reversible switched from anion to cation by changing the potential applied to the conductive membrane surface. Similar results were obtained for membranes prepared from alumina nanofibers with conductive carbon coating [2,3] as well as single nanochannels [4]. Note that the transport of charged species through

conductive nanopores can induce a surface charge via polarization effect, and thus alter the pore transport characteristics [5,6].

In this work, we have developed a hierarchy of mathematical models for describing ion transport in conductive nanopores. They are based on Navier-Stokes, Nernst-Planck, and Poisson equations, which are solved in a cylindrical nanopore geometry. The models are characterized by dimension (2D and 1D), boundary conditions (constant surface potential or constant total charge), external driving force (concentration or electrical potential gradient), the presence/absence of Stern layer. The software package for calculations and experimental data processing with the help of suggested models is developed. It is shown that the models can correctly describe the experimental data on the variation of membrane potential by external potential applied to the membrane surface [1,3] as well as the results on ionic conductivity of carbon nanotubes [7]. The non-linear behavior of current-voltage curves in nanotubes is explained by polarization of their surface by electric field and the corresponding redistribution of charge inside the nanotube.

The work is supported by the Russian Foundation for Basic Research Grant no. 18-38-20046.

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Theoretical and Experimental Investigations of Electroosmotic Flow Beyond Debye-Hückel Regime

Authors

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Abstract

Electroosmotic flow in the Debye-Hückel regime is well-studied in the literature. Our group also investigated electroosmotic flow in this regime using theoretical (molecular dynamics and continuum transport perspectives) as well as experimental methods. However, beyond Debye-Hückel regime, recent molecular dynamics studies have revealed charge inversion within the electrical double layer and flow reversal phenomena with progressive increase in the surface charge or in the wall potential. In this study, we provide an improved picture on electroosmotic flows beyond the Debye-Hückel regime, namely in the intermediate and flow reversal regimes using molecular dynamics simulations. To support the molecular dynamics findings, we also develop a continuum model based on Poisson-Fermi and Stokes equations including the overscreening and crowding effects, local variation of the viscosity and slip lengths. After extracting the continuum parameters from molecular dynamics

simulations, good agreement between simulation results and continuum predictions are obtained for surface charges as large as -0.37 C/m^2 . To validate our theoretical findings and truly assess electroosmotic flow beyond the Debye-Hückel regime, an experimental setup and protocol are developed, and experiments are conducted. Indium tin oxide (ITO) embedded electrodes which are isolated from an electrolyte by a silicon dioxide (SiO_2) dielectric layer are employed as active, tunable gates to systematically modify the local surface charge density at the electrode/electrolyte interface. A current monitoring method in which one electrolyte displaces another of different conductivity in a Y shaped microfluidic channel is implemented. The axial electric field, forming between the inlets and outlet, sequentially drives the ionic solutions through the microchannel. An independently controlled potential applied to the gate electrodes change the local surface charge density at the dielectric-electrolyte interface, enabling field-effect control over ionic transport, quantified by changes in the surface potential.

Molecular dynamics study of nanostructure formation of imidazolium-based ionic liquids with long-alkyl chains

Authors

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Abstract

Molecular dynamics simulations are performed on a 1-dodecyl-3-methylimidazolium hexafluorophosphate ($[\text{C12mim}][\text{PF}_6]$) ionic liquid using a united-atom model. The ionic liquid exhibits second step relaxation at temperatures below a crossover point, where the diffusion coefficient shows an Arrhenius to non-Arrhenius transition. Annealing below this crossover temperature makes an isotropic to (liquid-crystalline) mesophase transition, where the smectic A phase or crystal-like smectic B phase forms. Hundreds of nanoseconds are required for completing these transitions. A normal diffusion

process is found for anions along the layer-normal and -lateral directions in the SmA phase, but only in the lateral directions in the SmB phase. We find a preserved orientational order for the imidazolium-ring rotational and the alkyl-chain reorientational dynamics in both of the smectic phases.

Ref) Hailong Peng, Momoji Kubo, and Hayato Shiba, Phys. Chem. Chem. Phys. 20, 9796-9805 (2018). [selected for themed collection: 2018 PCCP HOT Articles]

Self-similar interfacial impedance of electrodes in high conductivity media

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Abstract

Most bioanalytical technologies utilize locally applied electric fields induced by miniaturized electrodes. Sensitivity and effectiveness of these electrodes are susceptible to electrode polarization (EP) at the electrode/electrolyte interface. EP increases with decreased electrode size and increased electrolyte conductivity (σ), and can dominate the impedance spectrum in 1 Hz to 1 MHz range. For example, microfluidic sensors that measure dielectric properties of biological cells suspended in physiological buffers ($\sigma \sim 1.5$ S/m) are overwhelmed by EP up to 1 MHz, overshadowing the crucial β -dispersion frequency range. Similarly, dielectrophoresis (DEP) based biological-cell capture/separation devices become inadequate typically above S/m, and this problem is further amplified by reduction in the electrode size. In this study, interfacial impedance is investigated considering the effects of electrode size, channel height, electrode surface morphology, and electrolyte concentration on characteristic time scales in a binary electrolyte using disk electrodes in both single electrode and parallel plate electrode configurations. Experimental results revealed self-

similarity of normalized impedances as a function of the dimensionless frequency. Numerical and analytical results obtained by solving unsteady fully coupled Poisson-Nernst-Planck equations show the similar behavior with those attained with experiments. Moreover, fern-leaf like hydrophilic fractal gold nanostructured porous electrodes are fabricated using electrochemical deposition technique. The impedance spectra measured with nanostructured electrodes also collapsed on impedance curves obtained with planar electrodes by multiplying dimensionless frequency with a coefficient. This coefficient is considered as a function of electrode surface property including porosity, thickness of nanostructures, tortuosity, or combination of these parameters. However, the importance of these properties could not be differentiated due to the morphological complexities of the fractal nanostructures. To identify this coefficient, surface of planar gold electrodes was covered with cylindrical nanorods with known height, diameter, and separation distance using template assisted electrochemical deposition approach. Current findings describe the coupled effects of electrode diameter, channel height, electrolyte concentration, and electrode surface morphology on the interfacial impedance spectra.

Theoretical and experimental investigations of self-similar interfacial impedance of disk electrodes in high conductivity media

Authors

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Abstract

Understanding the time-dependent formation of electric double layer (EDL) in response to varying external effects is a fundamental problem in electrochemistry, colloid science, biophysics, and micro/nanofluidics. Usually EDL formation causes nonuniform change of electrical behavior at the

electrode/electrolyte interface and is often considered to be the most possible reason for electrode polarization effect. In this study, the physics of EDL forming on an electrode immersed in a symmetric binary electrolyte and subjected to a small external AC voltage is investigated. The Poisson–Nernst–Planck equations are simplified to Debye-Falkenhagen equation considering the linear regime. Analytical solutions are obtained for the space charge density and impedance of the system. Depending on the Debye length, λ_D , and the electrode separation distance, L , EDL charging time scales for binary electrolyte with the ionic diffusion coefficient of D is attained as $\tau_{c1} = \lambda_D L / D$ for parallel plate electrode configuration. On the other hand, the primary characteristic time scale is obtained as $\tau_{c2} = \lambda_D \Phi / D$ for a single disk electrode configuration, where Φ is the electrode diameter. We propose a dimensionless analytical expression for the impedance of electrode/electrolyte system, which can predict the experimental and numerical results. Normalizing the impedance magnitude with the solution resistance, and making the frequency dimensionless with the characteristic time scale for thin EDL, all analytical, experimental, and numerical data collapsed on to a universal curve. Moreover, universal space charge density equation is obtained for various solution conductivities and electrode separation distances. Based on the impedance spectroscopy results, one can attain the corresponding space charge density at an applied AC potential.

Study of Ion Transport Through A Two-Dimensional Porous Charged Interface

Authors

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Abstract

In our work, we investigate ion transport through a monolayer perforated graphene membrane. The study is important in fundamental understanding of

transport behavior of ions through a two-dimensional nanoporous charged interface as study of two-dimensional materials are emerging and limited number of studies have been reported on the ion transport behaviour of these materials. Ion beam bombardment was used to create nano pores in graphene supported on polymer foil (Madauß et al., *Nanoscale*, 2017, 9, 10487–10493). The pores in the supported polymer are much larger than the graphene pores to minimize any potential impact of the support structure. Measuring the induced potential across a charged interface using both mono and multivalent salts with a constant electrolyte concentration ratio provides a direct understanding of the selectivity and thereby the ion transport behaviour through the membrane. Our experimental results show that at low electrolyte concentrations, the potential enters into a Donnan regime where the potential is constant vs. concentration at a fixed concentration ratio between compartments. With increasing concentration, eventually the potential decreases and at high salt concentrations, the potential could be related to the induced diffusion potential dominated regime resulting from the difference in mobilities of cations and anions in the membrane (Ghosh et al., *J. Phys. Chem. Lett.* 2018, 9, 6339–6344). This behaviour in a two-dimensional membrane like graphene is similar to that observed for dense ion exchange membranes, which is well described by the Teorell-Meyer-Sievers (TMS) relationship. However, for these graphene membranes the Donnan potential value at low concentrations is less than the theoretical Nernst potential. This could arise from defects in the graphene layer, low surface charge or the inability of a continuum model to describe this 2D nanoporous system. The fitted parameters of the modified TMS model indicates a low value of fixed ion concentration compared to the dense membranes, implying a low value of surface charge for a single layer graphene. The ratio of diffusion coefficients of cations and anions are consistent with their bulk value which is not a typical characteristic of a dense ion exchange membrane. This investigation reveals some of the fascinating features of ion-transport across 2D membranes and opens up exciting opportunities for further understanding of transport in such atomistically thin interfaces.

A novel electrochemical flow sensor using the convective-diffusive ionic concentration layer by ionic concentration-polarization

Authors

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Abstract

We present a novel flow sensor based on electrochemical sensing of the ionic concentration-polarization (CP) layer developed within a microchannel-ion permselective membrane device. To demonstrate the working principle of the electrochemical flow sensor, the effect of advection on the transient and steady-state ionic concentration-polarization (CP) phenomenon in microchannel-Nafion membrane systems is studied. For this, we designed, fabricated and tested a unique microfluidic device with sensing electrodes embedded within the microchannel and with powered electrodes (anode/cathode) within the inlets of the microfluidic channel and of the side channels. We examined flow-sensing using both local transient impedance measurements, using an array of sensing electrode pairs, as well as global current measurements (I - t) across a membrane (i.e., between electrodes inserted at the inlets of the main and side microchannels). In the former, we analyzed the time-of-flight and the steady-state impedance value versus flow rates, both of which showed a strong dependency on the flow rate, with the latter being more robust (i.e., linear dependency on the flow rate). The global I - t measurements also demonstrated a strong dependency of both the time to steady-state as well as the value of the impedance on the flow rate. These local and global electrical measurements were conducted under either step-wise application of CP under steady-state flow or step-wise application of flow (i.e., pulsative flow conditions) under steady-state CP. All of the above tests proved the capability of the sensor to robustly measure small flow rates.

Electroneutrality breakdown in nanopores: a 1d mean-field theory

Authors

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Abstract

Ion transport in extremely narrow nanochannels has gained increasing interest in recent years due to its unique physical properties, and the technological advances that allow us to study them. It is tempting to approach this regime with the tools and knowledge developed for wider microfluidic devices, and use continuum models like the Poisson-Nernst-Planck equation. However, it turns out that some of the most basic principles we take for granted in a large system, such as electroneutrality, can breakdown under extreme confinement. We show that in a truly one-dimensional system, interacting with three-dimensional electrostatic interactions, the screening length is exponentially large in ionic spacing, and can easily exceed the macroscopic length of a nanotube. Without screening, electroneutrality is broken, and ionic transport can behave in a completely different way. In this work, we build a theoretical framework for electroneutrality breakdown in a one-dimensional nanopore and show how it provides an elegant interpretation for the peculiar scaling observed in experimental measurements of ionic conductance in carbon nanotubes.

Electric Field Driven Characterization of Biovesicles

Authors

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Abstract

Cell derived vesicles such as endosomes, exosomes, and lysosomes are natural carriers for the transport of biological cargo in and out of cells. Consequently, sub-micron scale bioengineered vesicles hold immense promise as one of the

safest and most effective carriers for drug transport in living organisms. However, due to the structural differences in bioengineered vesicle membranes, theoretical models developed for biological cell membranes perform poorly in predicting dynamic behavior of bioengineered vesicle. In this study, we investigated the dynamic landscapes of bioengineered vesicle electrodeformation by coupling shear flow and electrophoretic forcing mechanisms using an interface resolved framework. The immersed interface method is used to solve the electric field, while the immersed boundary formulation is used to resolve the fluid-structure interaction with deforming and translocating vesicles. Modifications to membrane model is proposed to capture behavior of bioengineered vesicles. Significantly, we find a high rate of areal dilatation for artificial (lab-derived) vesicle membranes. Our model results show that membranes remain stable up to 15% change in surface area. Depending on the shear rate and applied electric field, tumbling and tank treading motions are observed. Model results also show that composite domain conductivity can be used as a good metric to detect vesicle movement and the extent of deformation. This electric field driven mechanism shows significant prospect as an effective non-intrusive method to characterize the properties and deformation dynamics of bioengineered vesicles.

1D and 2D modeling of electrodialysis and reverse osmosis

Authors

Dr. Maarten Biesheuvel - Wetsus

Abstract

The Sonin-Probst approach (MIT, 1968) is a very elegant and powerful method to describe a full 2D electrodialysis device, and it is relatively easy to program. Its key feature is to assume that along the membranes we only have to consider advection, and for long and thin channels this is a highly accurate assumption. This simplification allows incorporating important other modelling elements in much detail, such as ion-ion and ion-wall frictions in membranes, as well as acid-base equilibria between ions, and the equilibria of ions with the membrane wall charge. Water flow through the membrane can also be included. In this approach, the concept of the “concentration polarization layer”, or

“diffusion boundary film” next to the membrane becomes obsolete, and instead is resolved without having to specify a thickness for that virtual layer.

For reverse osmosis, we use a modified Nernst-Planck model to describe data for a multicomponent mixture of ions, focusing on all acid-base equilibria that occur, which are influenced by local pH in the membrane. Prediction of pH in the membrane and in the effluent is a natural part of the model. This model extension is very relevant when water contains ions that exist in multiple charge states, like ammonia/ammonium, borate ion/boric acid and the three carbonate species.

In membrane-based desalination, heat effects are important. In most cases, the water will slowly heat up because of conventional Joule heating due to the resistance to electrical current. However, as already identified in 2014, in an ion-exchange membrane process, at some positions there must also be cooling. We present our theoretical and experimental results of the temperature developments on opposite sides of an ion-exchange membrane, and show how indeed at one membrane face the water is cooling down.

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Numerical Simulation of Electrothermoplasmonic Flow around an Array of Gold Nanoantennas for Enhanced Plasmonic Sensing

Authors

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Abstract

Plasmonic-based biosensors have emerged as a powerful, cost effective and portable platform for pathogen and biomarker detection. In particular, Localized Surface Plasmon Resonance (LSPR) based systems, which rely on resonance shift tracking, present high sensitivity, specificity and real time detection. Current approaches integrate the plasmonic sensors in microfluidic channels, providing a multiplexing platform where many different experiments can be run in parallel [1]. Although promising, the performance of such approach is strongly limited by the long experimental times imposed by the diffusion-limited transport of the species. Consequently, a large amount of them do not interact with the sensor, leading to long assay times and a waste of sample. In recent years, researchers have investigated a variety of approaches to solve this general and crucial issue, using optofluidics [2, 3] and electrokinetics effects [4].

Here, we present numerical simulations of the laser-induced heating of a single or array of gold nanoantennas which, in conjunction with an applied a.c. electric field, initiates rapid microscale fluid motion, termed electrothermoplasmonic (ETP) flow [5,6], and particle transport. The physics of the ETP flow mechanism is described by several coupled partial differential equations, which can be solved numerically using the Comsol Multiphysics software package. The numerical

results are compared with experimental measurements and are also used to explore the influence of the different geometries for the nanoantennas array and the parameters of the external applied electric field. The conclusions can help in the future design of optimized lab-on-a-chip devices.

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Electroconvection instability and deionization shock in a circular microchannel

Authors

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Abstract

Electrokinetics plays an essential role in desalination, electrochemical energy storage, and biomedical applications. Exploring various geometry or designing sophisticated structures is one of the typical approaches to actively control and manipulate ion transport, enabling the discovery of many rich physical phenomena. In this talk, electrokinetics in a circular microchannel is explored by the direct visualization of spatiotemporal evolution of flow and concentration. Electroconvection-driven deionization shock is identified, which propagates radially outward up to millimeter scales. Moreover, the equilibrium electroconvection instability will be discussed in this geometry as well. These results provide more opportunities to manipulate ion transport in complex geometries for desalination and water treatment.

Electrodynamics of particle compaction in electronic ink

Authors

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Abstract

In the field of electronic paper there is a lot of interest in an electrophoretic ink display with video-speed capability. To speed up such displays, switching of pigment particles must happen over shorter distances and in thinner devices, making particle-surface interactions more important.

Here, we investigate the compaction of pigment particles at the liquid-surface interface due to an applied voltage difference, in the regime of high particle and high surfactant concentrations. We combine transient electrical current measurements with reflectivity measurements based on total internal reflection. The former gives insight in the charge distribution where the latter gives us insight in the pigment particle concentration near the surface.

Experiments are carried out with an electrophoretic ink based on pigment particles in a fluorochemical fluid inserted between two glass substrates separated by 25 micrometer spacers. The substrates are covered with an ITO electrode and a dielectric coating of the poly(p-xylylene) polymer Parylene C with a thickness of 50 or 200 nm.

Transient current measurements show capacitive screening over the dielectric Parylene C coating. The total internal reflectivity shows a two-stage dynamical switch when the applied voltage is increased or decreased stepwise. The steady state reflection is high for negative voltages and low for positive voltages, with a characteristic transition at 3 V.

Based on an analytical model including positive pigment particles, negative inverse micelles and dielectric coatings, we can clarify the capacitive screening over the dielectric coatings resulting in accumulation of pigment particles at one side and accumulation of inverse micelles at the other side. With the addition of positive, fixed surface charge on the dielectric coatings we can also explain the observed steady state reflectivity as a function of applied voltage with its characteristic offset. With finite difference time domain simulations based on drift and diffusion we can reproduce the full two-stage switching and the asymmetric reflection reduction.

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Graphitic Carbon Nitride Impregnated Niobium oxide (g-C₃N₄/Nb₂O₅) Type (II) Heterojunctions and its Synergetic Solar-Driven Hydrogen Generation

Authors

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Abstract

Graphitic carbon nitride (g-C₃N₄) based catalysts are evolving in energy harvesting applications due to their robustness, nontoxicity, and most important photocatalytic efficiencies. In this work, we successfully engineered g-C₃N₄/Nb₂O₅ type (II) heterojunction via pulse sonochemical technique based on opposite charge-induced heteroaggregation on the surface. The agglomerated spherical Nb₂O₅ nanoparticles (NPs) having diameter 30–40 nm observed on the lamellar surface of g-C₃N₄ in FESEM images. The XRD and XPS analysis confirm the orthorhombic phase and formation of the g-C₃N₄/Nb₂O₅ heterostructure. The FTIR spectra of g-C₃N₄/Nb₂O₅ show characteristic poly-s-triazine bands from 1250 to 1650 cm⁻¹. Moreover, g-C₃N₄/Nb₂O₅ exhibited the lower bandgap value of 2.82 eV as compared to Nb₂O₅ (3.25 eV) with significant redshift and enhance visible light absorption. The Mott–Schottky (MS) analysis confirms the formation of heterojunction between g-C₃N₄ and Nb₂O₅, with significant band shifting toward lower hydrogen evolution reaction (HER) potential. The g-C₃N₄/Nb₂O₅ heterojunctions showed many folds enhanced photocurrent response from photoelectrochemical (PEC) water splitting, and the value reached to -0.17 mA/cm² with good stability and insignificant dark photocurrent at 1.0 V vs RHE. The electrochemical impedance spectroscopic (EIS) measurements further elucidate the suppression of photogenerated electrons/holes as the radius of the semicircle significantly decreased in case of heterojunction formation. The enhanced photocatalytic hydrogen generation by the heterostructures could be attributed to the effective formation of heterojunctions between the g-C₃N₄ and Nb₂O₅ semiconductors, causing the migration of the photogenerated electrons and holes, hence increasing their lifetimes.

Theoretical Analysis of Electrochemically Mediated Selective Adsorption for Water Treatment

Authors

Ms. Fan He - Massachusetts Institute of Technology

Prof. Martin Bazant - Massachusetts Institute of Technology

Prof. T. Alan Hatton - Massachusetts Institute of Technology

Abstract

Water treatment by electrosorption is a topic of increasing interest in recent years due to the high efficiency, low cost, small footprint and no secondary treatment required compared with tradition water treatment methods, such as reverse osmosis and multi-stage distillation. Electrochemically mediated selective adsorption, is one of the emerging electrosorption techniques, which has drawn great attention recently. The great advantage of this technique is its superb selectivity (>100), which allows selective removal of high-valued or toxic target ions under low energy consumption, which is difficult to achieve by any other water treatment techniques.

Here, we develop a theoretical framework to study the multi-component mass transport phenomena within the electrosorption cell from first principle with no fitting parameters. The model coupled diffusion, convection and electromigration together with competitive surface adsorption reactions which are derived from thermodynamics. Due to the inherent complexity, a transient two-dimensional model is required to accurately describe the process in general. This allows a better understanding of the mass transfer behavior of the system and provides guidance on how to interpret the experimental data.

Through analytical derivations and numerical simulations, we demonstrate that under convection limited regime, which is achieved when the propagation of the target anions is the limiting step, mass transport in the electrosorption cell exhibits a moving front kinetics similar to the transport in chromatographic columns or packed bed adsorption.

A reduced order model is also derived from the governing equations to allow easier computation. A wave velocity and width are derived by a combined analytical and numerical approach, which can be used for reactor design, process optimization and scaling up.

The framework developed here provides a criteria for designing and operating continuous microfluidic devices based on diffusion, convection, electromigration and reaction of multiple competing ions under electric field. And have

applications not limited to electrochemical water treatment, but also in energy storage, microfluidic reactor design and bio-sensing, etc.

Elastic instability in soft microfluidic configurations driven by non-uniform electro-osmotic flow

Authors

Mr. Evgeniy Boyko - Technion-Israel Institute of Technology

Prof. Moran Bercovici - Technion-Israel Institute of Technology

Prof. Amir D. Gat - Technion-Israel Institute of Technology

Abstract

Non-uniform electro-osmotic flow (EOF) in microfluidic configurations gives rise to internal pressure gradients. In soft devices, these internal pressures can result in elastic deformation, thus yielding viscous–elastic interaction. In this theoretical work, we analyze the deformation instability of a pre-stretched elastic sheet separated from a rigid flat surface by a thin liquid film and subjected to non-uniform EOF. Applying the lubrication approximation to the flow field and modeling the elasticity using the linearized Föppl–von Kármán equations, we derive a nonlinear viscous–elastic governing equation describing the deformation of an elastic sheet, representing the balance between viscous and elastic resistances as well as an electro-osmotic forcing. Our theoretical analysis, validated by numerical simulations, reveals that the instability is controlled by a non-dimensional parameter representing the ratio of electro-osmotic to elastic forces, and also indicates the existence of hysteresis for the onset of instability. We consider both a constant voltage and constant current actuation modes and examine the elastic instability under various bending and tension conditions, demonstrating that the elastic sheet exhibits distinct modes of instability depending on the electro-osmotic pattern. Furthermore, this instability can result in a non-symmetric deformation pattern, even for symmetric actuation. The mechanism illustrated in this work, together with the provided analysis, may pave the way for implementation of instability-based soft-actuators.

Modeling of Direct Current Electrokinetic Motion of Janus Particles and Droplets

Authors

Mr. Atakan Atay - Bilkent Univerisity

Prof. Barbaros Cetin - Bilkent Univerisity

Prof. Ali Beskok - Southern Methodist University

Abstract

Electrokinetic manipulation of Janus particles/droplets has attracted attention in recent years due to their potential application in microfluidics. Due to the presence of two different zone on the surface of particles with different charge distribution, the motion of the Janus particles is quite different than that of homogeneous ones. Therefore, fundamental understanding of this motion is the key element for further development of microfluidic systems with Janus particles. Electrokinetic motion of particles can be properly modeled using the stress tensor approach, which considers the finite particle size, and particle-particle and particle-surface hydrodynamic and electrokinetic interactions. In this approach, the drag and electrokinetic forces and torques acting on the particles are obtained by integrating the hydrodynamic stress tensor, and Maxwell stress tensor, respectively. Volume based numerical models are faced with algorithmic and computational challenges in resolving complex particle shapes and in efficient implementation of particle motion. In addition, resolution of hydrodynamic and electrokinetic interactions between close particles and surfaces often require unusually high mesh density. These challenges are eliminated by using the Boundary Element Method (BEM) that requires discretization of the particle and channel surfaces, which effectively reduces 3D problems to 2D, and 2D problems to 1D. We recently developed a 2D BEM for simulation of particulate flows in the Stokes flow regime. The algorithm properly captures electroosmotic flows, electrophoretic and dielectrophoretic responses of multiple particles. In the present study, DC electrokinetic motion of Janus particles and droplets inside a micro-channel is modeled using boundary element formulation with the assumption of thin electrical double layer. 2D

formulation is verified against the reported experimental data in the literature. Results show that the 2D boundary element formulation is successful for capturing physics of particle flow and prediction of the electrophoretic velocity of the Janus particles and droplets. Following the verification of the model, some important aspects of electrokinetic motion Janus particles/droplets will be presented including the cases with particle-wall and particle-particle interactions.

Structure and Dynamics of Electrical Double Layers in Thin Brine Films

Authors

Mr. Chao Fang - Virginia Tech

Prof. Rui Qiao - Virginia Tech

Abstract

The wettability of oil on rock surfaces plays a crucial role in their recovery from reservoirs. In both sandstone and carbonate reservoirs, a thin brine film often exists between oil droplets and rocks, and the wettability of the oil droplet depends on the disjoining pressure in this brine film, which in turn depends on the electrical double layers (EDLs) in the thin brine film. In this work, we study the EDLs in thin brine films using molecular and continuum simulations. We first examine the structure of the EDLs in terms of water and ion distributions and the orientation ordering of water molecules across the films. The evolution of the EDL structure with the thickness of the brine film is highlighted. We next examine the relaxation dynamics of ions in the thin films and rationalize the observed dynamics by developing simplified models. The technical implications of the structure and dynamics of EDLs revealed in these simulations will be discussed.

Equilibrium Electro-convective Instability in Electrodeposition with Butler-Volmer Kinetics

Authors

Prof. Isaak Rubinstein - Ben Gurion University of the Negev

Prof. Boris Zaltzman - Ben Gurion University of the Negev

Abstract

In this presentation we report that equilibrium electro-convective instability is possible in concentration polarization in the course of cathodic electrodeposition. The cathode is modeled as an ideally perm-selective interface with infinite lateral conductivity. The cation transfer across the cathode/solution interface is assumed to obey the Butler-Volmer kinetics with parameters typical of copper deposition. It is shown that deviation from the local reaction equilibrium due to the final deposition reaction rate renders possible the equilibrium electro-convective instability with a critical wavelength on the scale of diffusion layer width. This scaling may be recognized as a characteristic signature of equilibrium instability as opposed to the non-equilibrium one, related to the extended space charge. This latter instability, owing to its shortwave character, is characterized by origination of critical small vortices with a wavelength considerably shorter than the width of the diffusion layer. Interaction of these small scale vortices yields their fusion through which they evolve until reach a size comparable to the width of the diffusion layer.

Unexpected surface forces generated by the action of electric fields across ionic liquid electrolytes

Authors

Dr. Carla Perez Martinez - University of Oxford

Prof. Susan Perkin - University of Oxford

Abstract

The application of electric fields across liquid films is ubiquitous in nature and technology, for example in cell membranes, liquid crystal displays, and energy storage. Here we explore the force generation and surface interactions when electric fields are applied across fluid films. A surface force balance (SFB) is used to measure directly the force between two electrodes in crossed-cylinder geometry across thin films of dielectric and electrolytic fluids. Electrolytes display unexpectedly strong and slow responses under application of an AC electric field.

In the SFB, white light interferometry is used to determine the thickness of the liquid separation; by applying a voltage to the mirrors of the interferometer, an electric field can be applied to the liquid of interest. We have measured the interaction force between electrode surfaces as a function of their separation distance and applied voltage, across a non-polar oil (polydimethylsiloxane), used as a control, and two ionic liquids. Both the transient forces after switching the applied field and the steady-state interaction force between the surfaces were measured, and we compare the results to calculations of the equilibrium and transient forces in the system. We find that measurements with the dielectric fluid match closely to the calculated behaviour for DC and AC fields, during the transient and at steady state, with no fitting parameters. The timescale for the response is dominated by hydrodynamic drag.

When the test liquid is an electrolyte, an alternating electric field induces a force which diverges substantially from the calculated static response of the electrolyte. Thin films of two ionic liquids, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide, were studied. The magnitude of the force measured with these liquids is several times larger than predicted, and the interaction can switch from attractive to repulsive. Furthermore, the approach to steady state in electrolyte is slow (of the order of 10^3 s), compared to both the charging and viscous timescales of the system. The magnitude of the force seems to be independent of the liquid film thickness (varied between 8-64 μm) and AC field frequency (10^2 - 10^6 Hz), but scales with the square of the applied voltage amplitude. When the electric field is switched off, the system response is

reversed, and the system relaxes back to its original state in an equally slow timescale. We will also report on measurements using mixtures of ionic liquid in polar solvent and aqueous electrolytes.

Our measurements provide a direct measure of the length- and time-scales relevant in AC electrochemical and electrokinetic systems, and they also suggest ways to control colloidal and soft matter using electric fields.

Electroconvection in membrane systems: experiment, modelling and applications to electrodialysis

Authors

Prof. Victor Nikonenko - Kuban State University, Membrane Institute

Abstract

In conventional electrodialysis (ED), target transport is the ion transport under the action of an applied electric field. In electrokinetic devices, such as micropumps, the goal is volume/fluid movement. The use of electroconvection, which is current-induced volume transport when an electric field is imposed through the charged solution, opens a new innovative kind of electrodialysis: ED in overlimiting regime, where current-induced volume transport is as important as ion transport. The operation in this regime allows a multifold increase in the rate of demineralization compared to conventional ED, where the current density is prescribed to be lower than the limiting current density.

According to classical electrochemistry, the rate of electrode and membrane processes, at least in dilute solutions, is limited by the diffusion-controlled “limiting” current density, i_{lim} . The breakthrough was made by pioneering paper of Rubinstein and Shtilman [1]. They showed that the useful current density can be greater than i_{lim} due to a reduction of the diffusion boundary layer, which is destroyed from the edge contacting the membrane. Later a significant number of papers were devoted to establishing the mechanisms of electroconvection, which destroys the diffusion layer from the inside, so that the layer where

diffusion is dominant shrinks and moves from the membrane surface to the bulk solution.

This presentation gives a review of experimental results and simulation showing a strong relationship between the intensity of electroconvection and the surface properties of ion-exchange membranes. It is established that there is an optimum distribution of conductive and non-conductive surface areas, when the mass transfer rate reaches its maximum under a given voltage due to intensive electroconvection. However, it is not clear how this optimum distribution depends on the conditions of electrodialysis, such as solution flow rate and intermembrane distance. An important issue is water splitting and membrane fouling, which both can be reduced by electroconvection. Chemical composition and electrical heterogeneity of membrane surface affect essentially the water splitting rate. It is possible to reduce significantly water splitting by grafting functional groups, which have nearly zero catalytic activity towards this reaction. However, it is not possible to suppress it totally. As it was shown recently, water splitting always occurs in the extended space charge region, while with a rate constant proper to free solution not affected by catalytic processes. At very high voltages the thickness of this region attains several microns, then water splitting rate becomes significant.

Along with analysis of electroconvection mechanisms, a number of valuable applications of electroconvection in ED are discussed in literature. Among them are shock ED [2] and ion concentration polarization ED, where only ion-selective membranes of unipolar conduction are used [3].

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Chronopotentiometry of heterogeneous ion-exchange membranes with hydrophobic or hydrophilic non-conductive surface areas: 2D simulation

Authors

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Prof. Victor Nikonenko - Kuban State University, Membrane Institute

Abstract

Introduction

Heterogeneous ion exchange membranes are widely used in electrodialysis. It is well known that their electrically heterogeneous surface stimulates electroconvective mixing of the solution on the membrane diluate side at overlimiting current densities [1]. Davidson et al. [2] theoretically showed that the heterogeneous membranes with specified surface tailoring can possess mass transport characteristics exceeding homogeneous membranes. The determination of precise fraction of insulating surface and other parameters affecting the mass transport, such as hydrophobicity, is required for such improvements. The aim of the work is to show the effectiveness of membrane surface hydrophobization for the mass transport improvement.

Modelling

The conventional equations system (Nernst-Planck-Poisson-Navier-Stokes) of the basic mathematical model [3] is applied when using the approach of electric current stream function [4] to simulate the ion and volume transport in an electrodialysis system with a heterogeneous membrane. The model is two dimensional and nonstationary. An anion-exchange membrane whose surface consisted of alternating conductive (10 μm wide) and insulating (40 μm wide) stripes was examined.

Two extreme cases were studied. In the first case (denoted as “hydrophobic membrane”) the insulated stripes were assumed hydrophobic, which did not hinder the slip of fluid; the slip boundary condition was applied. In the second case (“hydrophilic membrane”), these strips were assumed hydrophilic; the non-slip boundary condition was applied.

Results and Discussion

The shape of numerically simulated chronopotentiograms (ChPs) allows distinguishing three regions, differing in the mode of ion delivery to the membrane surface. In the first one, no difference can be observed between ChPs and concentration profiles for hydrophobic and hydrophilic membranes. The dominant mechanism of ion delivery is electrodiffusion.

The second region is characterized by a steep increase of potential drop with time caused by depletion of the solution at the membrane surface. The ChPs of hydrophilic and hydrophobic membranes become differing. The concentration profile of counterion near the hydrophilic membrane is almost linear, meaning that, due to absence of fluid slip, the main mechanism of ion delivery is still electrodiffusion. A lower potential drop and strongly nonlinear concentration profile near the hydrophobic membrane show that the mechanism of ion delivery becomes mixed. However, the contribution of electroconvection is weak and occurs only close to the membrane surface near the conductive stripes. The hydrophilic membrane shows such a behavior later, at transition time.

In the third region, smooth but quite significant growth of potential drop appears in both systems due to depletion of the solution near the conductive stripes. Then the potential drop steeply decreases and reaches a stationary value. Experimental ChPs confirm the behavior described above.

This study was realized in the frame of a joint French-Russian PHC Kolmogorov 2017 project with the financial support of Minobrnauki (Ref. N° RFMEFI58617X0053), Russia, and CNRS, France (project N° 38200SF).

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DIFFUSION-BASED SEPARATION USING BIDIRECTIONAL ELECTROOSMOTIC FLOW

Authors

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Dr. Federico Paratore - IBM Research - Zurich

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Abstract

We present an analytical and experimental investigation of a novel method that leverages non-uniform electroosmotic flow to achieve diffusion-based separation. We pattern the bottom of an unobstructed fluidic chamber with stripes of alternating surface charges, and upon the application of an external electric field parallel to the stripes, a bidirectional electroosmotic flow pattern is formed. The surface charge of each stripe is obtained by controlling the potential of an electrode array embedded in the floor of the microfluidic chamber and the potential in the chamber. High-diffusivity particles introduced into the bidirectional flow rapidly diffuse across stripes and experience an average zero velocity, whereas low-diffusivity particles remain on single stripes and therefore advect through the microfluidic chamber. We show experimental results of separation of low-diffusivity beads from high-diffusivity dye. To the best of our knowledge, the separation method presented in this work is the first demonstration of diffusion-based separation that is able to separate low-diffusivity species from mixtures without the use of mechanical components

(e.g. syringe pumps or pressure systems) and we believe this method could serve as an *in-situ* sample preparation step for lab-on-chip applications.

Non-uniform electro-osmotic flow drives elastic deformation instability

Authors

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Mr. Ran Eshel - Technion - Israel Institute of Technology

Prof. Amir Gat - Technion - Israel Institute of Technology

Prof. Moran Bercovici - Technion-Israel Institute of Technology

Abstract

In this theoretical and experimental work, we report for the first time the deformation instability of an elastic substrate separated from a rigid surface by a viscous liquid film subjected to a non-uniform electro-osmotic flow (EOF). We first provide insight into the physical mechanisms underlying the instability by considering a simplified 1D model, inspired by electrostatic MEMS actuators, in which the elastic substrate is modeled as a rigid plate connected to a linear spring. Our linear stability analysis, supported by experimental observations, reveals an instability that is controlled by a non-dimensional parameter representing the ratio of electro-osmotic to elastic forces, and also indicates the existence of a threshold value of the electric field for the onset of instability. To experimentally demonstrate the deformation instability, we fabricated a microfluidic device consisting of a fluidic chamber with an elastic upper sheet and a rigid bottom surface which is partially coated with a cationic polyelectrolyte to create a non-uniform surface charge. We placed a rigid plate on top of the elastic sheet and measured the gap between the two surfaces, resulting from negative pressures created by the non-uniform EOF. We determine the temporal evolution of the gap by measuring the three-dimensional point spread function (PSF) of micro-beads patterned on top of the rigid plate. We demonstrate that above a certain threshold of the electric field, the system exhibits instability, which collapses the upper plate onto the bottom

surface. Furthermore, using both theoretical predictions and experimental observations, we identify three distinct dynamic behaviors, which we refer to as (i) a stable steady state case, (ii) a bottleneck case, and (iii) an immediate collapse case. We believe that the mechanism illustrated in this work, together with the provided analysis and experimental demonstration, may prove valuable for the implementation of instability-based actuators.

CFD simulations of electrokinetic instabilities in electromembrane processes

Authors

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Abstract

In the field of water desalination and purification by electromembrane processes, understanding ion transport in overlimiting current regime is of high interest nowadays, in order to identify new applications (e.g., disinfection [1]), and exploit electrokinetic instabilities to enhance desalination performance [2]. Electroconvection phenomena arising near ion exchange membranes can be relevant in Electrodialysis (ED), membrane capacitive deionization, and other ED-related techniques such as Shock ED [1].

In this work, electroconvection phenomena were investigated by computational fluid dynamics (CFD) simulations by using a commercial code (Ansys CFX) [3, 4], where the Nernst-Planck-Poisson equations are coupled with Navier-Stokes equations, and solved without any simplifying assumptions. Electrokinetic instabilities were simulated for different computational domains (both 2-D and 3-D) and boundary conditions. In particular, we adopted the Okubo-Weiss parameter, which shows the relative contribution of vorticity versus shear, to have an effective visualization of vortices. A new dimensionless time was defined

to facilitate the comparison between simulations with different evolution time constants (i.e., time to reach a fully-developed regime). Results show how electroconvective vortices cover a large portion of channels and velocities attain relatively high values, increasing about linearly with the applied voltage.

Keywords: CFD, electroconvection, shock ED, electroconvective transport, overlimiting current.

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Electro-Optical Response of Graphene Oxide Dispersions under Alternating Fields

Authors

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Abstract

In this work, we analyse the electro-orientation of graphene oxide (GO) flakes in aqueous suspension in the absence of interparticle interactions, under different experimental conditions [1]. From the measurement of linear dichroism, the

electrical polarizability of the GO flakes as a function of the field frequency was calculated. The results show that the use of high frequency electric fields strongly enhances GO electro-orientation. These results shed light on recent studies on GO focused on applications such as the fabrication of transparent electrodes or drug delivery, since the interaction of this material with electric fields is yet poorly understood, and only recently the orientation of GO particles with an electric field was achieved [2].

Acknowledgements: Financial support of this investigation by Junta de Andalucía, Spain (grant No. PE2012-FQM-694) and University of Granada (Program 'Proyectos de investigación precompetitivos') is gratefully acknowledged. Thanks are due to Prof. A. Ramos, University of Sevilla, Spain for fruitful discussions.

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Electrokinetic trapping of anisotropic particles

Authors

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Abstract

In recent years anti-Brownian electrokinetic trapping has become a valuable tool in the study of individual particles and inter-particle interactions in liquid [1,2]. Electrokinetic trapping essentially uses real-time electrical feedback based on particle position measurements to largely eliminate the particle's Brownian motion. Besides enabling single particle studies for prolonged times while avoiding undesired interactions with interfaces, trapping can be used to characterize the diffusion coefficient, D , and electrophoretic mobility, μ , of particles in real-time by analysing the small deviations of the particle from the trap position. In such a way, prolonged measurements of individual particles can reveal detailed information and dynamics that cannot be obtained by ensemble-averaged measurements.

In this work, axial electrokinetic trapping of anisotropic particles in water is realized in devices with planar, transparent electrodes [3]. To achieve trapping in the axial direction, information on the axial particle position is required. Here, a trapping algorithm is developed which uses Fourier-Bessel decomposition of standard microscopy images and which is learning from the correlation between applied voltages and changes in the particle appearance. No previous knowledge on the particle appearance, theory fitting or advanced optical setup is required. The algorithm is demonstrated by axially trapping singlets, doublets and triplets of polystyrene particles in water.

To characterize the trap and to extract particle properties, the motion of a trapped particle is investigated in detail. The particle position depends on diffusion and electrophoresis in a time-dependent local electric field, on the feedback rate and on the delay time between position measurement and actual electrical feedback. The time-dependency of the electric field is related to the build-up of diffuse double layers which causes screening of the bulk field, and Faradaic reactions at the interfaces at higher voltages. By comparing the position spectrum of a trapped particle to a simulation model, those dynamics of the electric fields are examined, and estimations of the electrophoretic mobility and diffusion coefficient of trapped particles are obtained.

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Theory of simultaneous desalination and electricity generation via an electrodialysis cell driven by spontaneous redox reactions

Authors

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Abstract

Electrodialysis (ED) is a well-established water desalination technology in which desalination is driven by an applied electric field, which results in salt ion electromigration through alternating cation and anion exchange membranes.

We here propose a modification to existing ED cell driving it via spontaneous redox reactions occurring at the electrodes. Such a cell is distinct from classical ED as it does not require electricity, but rather requires solely chemical energy input in the form of redox active chemicals, and outputs both desalted water and electricity simultaneously. We extend ED theory in order to capture an ED cell driven by spontaneous electrode reactions, demonstrating and quantifying predicted simultaneous desalination and electricity generation. In the cell considered, an AEM and CEM are separated by a channel with flowing feedwater. On the opposite side of the AEM is an anode and flowing anolyte, while a cathode and flowing catholyte are on the opposite side of the CEM. To capture cell behavior and performance at steady state, we solve the species' Nernst-Planck equation coupled with the electroneutrality condition and

consider electrode activation and concentration overpotential losses. We consider non-ideal membranes to capture species crossover as well as electric potential, counterion, and coion concentration variations within the membranes. Our model elucidates key phenomena predicted to affect our ED cell, including that the cell current is limited by reactant starvation at the cathode, and that current and fluxes of the main current carrying ions scale as $x^{-1/3}$, where x is the coordinate in the direction of flow. Our model predicts that our cell achieves an order of magnitude reduction in the NaCl concentration of a 500 mM feed, while generating up to ~ 42 mW/cm² electrical power density. The main limitation of the cell as designed is a relatively high coion crossover flux through the AEM and CEM.

Direct determination of the electrophoretic mobility of individual micro- and nanoparticles

Authors

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Abstract

Micro- and nanoparticles are increasingly used in a variety of biomedical applications, such as drug delivery or biomedical detection. Knowledge on a particle-to-particle basis of the surface charge is useful for detailed characterization of particles and their interaction with the environment, for example, in biosensing, nanocarrier engineering and in studies of protein corona. One approach to characterize the electrical properties of individual particles is to measure the electrophoretic mobility in a microchannel. However, the electroosmotic flow (EOF) complicates such measurements and can be a source of error.

Here, we present an analytical technique which minimizes the contribution of EOF such that the electrophoretic mobility of micro- and nanoparticles can be directly measured on a particle-to-particle basis. In our approach we use a custom-built inverted microscope combined with a fast CMOS camera. Particles are dispersed in a microfluidic cell and illuminated with an LED. Only particles situated near the center of the cross-section of the microfluidic channel are measured. An AC field is applied, and particle displacements are recorded at a high frame rate. Image analysis is performed in post-processing to extract the electrophoretic mobility.

Simulations based on Navier-Stokes equations show that in the middle of a 400 μm high fluidic channel (ibidi μ -Slide VI 0.4, length 17 mm, width 3.8 mm) and at an applied AC frequency above 200 Hz, the contribution of EOF becomes negligible, allowing to directly measure the electrophoretic mobility. The approach is demonstrated for 500 nm particles on a particle-to-particle basis. The accuracy of the electrophoretic mobility values is analyzed by comparing particle mobility values at different AC frequencies and locations in the channel to the theory.

The effect of electroconvective instability on the transient response of a microchannel-nanochannel interface device

Authors

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Prof. Gilad Yossifon - Technion-Israel Institute of Technology

Abstract

The transient response of a 95 μm deep microchannel-nanochannel interface device exhibits a non-monotonic behavior. This non-monotonic signature differs from that of our previously studied 4 μm deep microchannel-nanochannel interface device [1] and occurs in much shorter times. The experimental chronopotentiometric (chronoamperometric) response shows a distinct minima (maxima) at times that shorten with increasing applied current (voltage) and

scales linearly with the inverse of the current squared indicating that it is related to the interfacial depletion, similarly to Sand's time [2]. Microscope visualization shows the development of vortices and depletion regions reminiscent of that expected as a result of electro-convection instability (EOI) [3]. These observations are complemented with numerical simulations indicating that indeed such a non-monotonic response corresponds to the existence of EOI [4].

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Electrokinetic Phenomena in Oil Recovery and Production: From Theory to applications

Authors

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Abstract

Crude oil is still the most readily exploitable source of energy available to us and the main source of feed-stocks in many industries and products. The natural subsurface system in which oil recovery and production processes take place involves a variety of moving charged interfaces, and thus rely intricately on the electrokinetic properties of that system's components. Furthermore, several key applications in oil recovery and production applications can significantly benefit from a number of electrokinetic phenomena that can be exploited downhole or in the reservoir. In this presentation, examples of such phenomena will be presented and discussed. One example is acoustophoresis employed to

separate oil and fines from water downhole and from produced water on the surface. In the second, diffusiophoresis, chemiphoresis, and solute-capillary flow are harnessed to deliver surfactants and oil tracers to oil-rich regions in the reservoir that are inaccessible to conventional waterflood.

Understanding coion transport and water dissociation in bipolar electrodialysis for energy storage applications

Authors

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Abstract

Bipolar membranes (BPMs) are commercially developed nowadays for the production of acid and base via bipolar electrodialysis (BPED), though a number of novel applications has been recently proposed (including, e.g., energy storage, and CO₂ capture). Ideally, a BPM should promote only the transport of water molecules inside the membrane, where the production of protons and hydroxyls take place due to water dissociation. However, other ions in solution will transfer through the BPM to some extent, thus affecting the pH evolution inside the membrane, and therefore the process performance. A fundamental understanding of ion and water transport in bipolar membranes is of high importance, especially nowadays that novel BPMs are needed for different applications.

The aim of this work is to investigate ion transport in bipolar membranes, taking into account the transport of electrolyte (e.g., NaCl) and the production of H⁺ and OH⁻ inside the membrane. We theoretically investigate the membrane behavior by adopting a model based on the Nernst-Planck theory [1–3], where the BPM is modeled as two ion-exchange layers with constant fixed charge density. In particular, the model uses only the membrane thickness and charge density as input parameters, and predicts the concentration profiles of four ions (Na⁺, Cl⁻, H⁺, OH⁻) inside the membrane. Interestingly, the model shows that the electrolyte bulk concentration significantly affects the pH evolution, due to the competing ion transport inside the bipolar membrane. Finally, we aim to understand the effect of salt concentration in the BPED process, to identify the

optimal range of operating conditions (i.e., current density, bulk concentration) for enhancing current efficiency and water dissociation in bipolar membranes.

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Induced Polarization Due To Dispersed Electronic Conductors in Brine-Filled Porous Media

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Abstract

Complex conductivity mapping has gained increasing attention over the past century or so, as a means of detecting the presence of geological materials such as clay, ore, pyrite and potentially hydrocarbon, embedded in a porous rock matrix filled with an electrolyte that otherwise dominates the overall conductivity. Complex conductivity in such materials is typically attributed to two distinct processes: “Electrode Polarization” caused by charge accumulation in the

electric double layer (EDL) of non-ionic conductors, and “membrane polarization” associated with the redistribution of ions in the electrolyte around ion-selective grains. Despite a long history of research and empirical use, neither of these mechanisms have been understood at a sufficiently fundamental level to be able to quantitatively predict the emergent complex conductivity based on microstructure. Instead, spectral complex conductivity measurements have been fitted to empirical functional forms, such as the Cole-Cole model, and attempts have been made to relate the fitting parameters to statistical parameters such as grain size, volume fraction etc. In fact, similar fitting functions have been used for either mechanism, despite the fact that they are governed by entirely different physics and that they exhibit distinct scaling behavior.

In this contribution, we tackle the first of these two mechanisms, due to the presence of compact, as well as porous, conductive inclusions. We establish a theoretical framework relating spectral complex conductivity in these systems to the geometry and intrinsic properties of the materials, based on insights provided by experiments on model systems that include spherical inclusions made of gold, stainless steel, activated carbon, etc. embedded in a spherical glass bead pack. We obtain quantitative agreement between experiment and theory, not just for characteristic frequencies and amplitudes, but for the entire spectral shape of the phase angle between electric field and current density.

Based on this insight, we infer that low frequency (0.1-10 Hz) induced polarization signatures observed in a geophysical setting can be caused by such conducting inclusions only if either a) the inclusions are massive, i. e., electronically connected at scales much larger than typical grain sizes, or, b) are nanoporous with very large specific surface area. We explore the potential for diagenetic processes such as bacterial sulfate reduction to create such nanoporous grains via biomimetic experiments, and look for evidence of natural occurrence of such nanoporous sulfides in Mediterranean sapropels.

Electroconvection at an anion-exchange membrane in NaH₂PO₄ and NaCl solutions

Authors

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Abstract

Electroconvection in ion-exchange membrane systems with a NaCl solution is a relatively well-studied phenomenon. This study is an attempt to assess the degree of electroconvection development at the surface of an anion-exchange membrane (AEM), which is bathed in a NaH₂PO₄ solution, which is an ampholyte. When the ions constituting NaH₂PO₄ interact with water, the molecular form of orthophosphoric acid (H₃PO₄) and multiply charged anions (HPO₄²⁻ and PO₄³⁻) as well as H⁺ / OH⁻ ions are formed. The composition of the solution depends on the pH value.

We conducted a 1D simulation of the transfer of molecular and ionic forms contained in a 0.02 M NaH₂PO₄ solution through an anion-exchange membrane. The model is based on the Nernst-Planck equations and the local electroneutrality assumption; a membrane and two adjacent diffusion layers are considered. The calculations, as well as the experimental determination of the partial fluxes of all species present in the membrane system, lead to the following conclusions. The protons are produced in the depleted solution due to partial dissociation of the HPO₄²⁻ anions, when they enter the membrane under the action of electric current. This process begins at current densities below the limiting current density, i_{lim} , and the concentration of H⁺ ions increases with increasing current density. As a result, protons become the dominant carriers of electric charge in the near surface solution in intensive current regime. The

visualization of the vortex structures, made in a flow-through cell in parallel with the measurement of current-voltage characteristics, shows that electroconvection occurs in such membrane systems. The difference compared to the NaCl case is that these structures are much smaller in NaH₂PO₄ solution, and they form at higher i/i_{lim} ratios. Apparently, the H⁺ ions generated on the diluate side of the membrane reduce the electric space charge in the depleted solution, which in turn reduces electroconvection. Nevertheless, the effect of electroconvection causes an increase in the total flux of phosphorus through the membrane, which is important in electrodialysis applications for the production of fertilizers.

We are grateful to the Russian Science Foundation, project № 17-19-01486, for financial support.

Propulsion of asymmetric dielectric particles under high frequency AC electric fields

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Abstract

Under an AC electric field that is applied perpendicularly between two electrodes, it has been shown that asymmetric particles can propel along the substrate due to a few different mechanisms. For example, metallodielectric Janus particles propel with the dielectric hemisphere leading due to the induced charge electrophoresis. On the other hand, dielectric dumbbells made from silica and polystyrene spheres can also move with the silica lobe leading due to unbalanced electrohydrodynamic flow. These particles typically move at frequencies below 10 kHz. We recently, however, discover that the same silica-

polystyrene dumbbells can also propel in the high frequency regime (~100 kHz - MHz), which is well beyond the charge relaxation time of electric double layer near the electrode. Interestingly, the propulsion direction of the asymmetric dumbbells at high frequency is opposite to that in the low frequency regime, i.e., the polystyrene lobe is leading. Our experiments with tracer particles further show that there is a strong and contractile hydrodynamic flow surrounding both silica and polystyrene lobes. In fact, the flow is so strong that the whole dumbbell, while propelling, is lifted at least ten microns beyond the substrate. The flow surrounding the polystyrene lobe is stronger than the silica lobe, which generates a net flow towards the silica lobe, consistent with the net propulsion direction towards the polystyrene side. We further show that this unbalanced electrohydrodynamic flow at high frequencies is a universal phenomenon not only applied for inorganic particles but also for biological cells such as yeast. By exploiting this flow, we build microscopic motors that can selectively bind, transport, and deliver specific types of cells among a mixture.

Temperature dependence of Diffusiophoresis

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Abstract

Diffusiophoresis can play an important role in the transport of colloids in confined geometries. However, many applications involve elevated temperatures and hence the effect of temperature on diffusiophoresis becomes important. The theory of diffusiophoresis is well established, but the effect of temperature on diffusiophoresis has not yet been investigated systematically and experimentally. In this work, we carry out experiments using a 3 – channel microfluidic device, with integrated hydrogel membrane windows to impose controlled electrolyte gradients. We systematically vary the system temperature and visualize and measure the diffusiophoretic migration velocity of model colloids, from which diffusiophoretic mobilities are determined and compared with the theory.

Active electrokinetic control of the concentration-polarization layer in a microchannel-ion-permselective membrane system

Authors

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Abstract

The ability to induce regions of high and low ionic concentrations adjacent to a permselective membrane or a nanochannel subject to an externally applied electric field (a phenomenon termed concentration polarization) has been used for a broad spectrum of applications ranging from on-chip desalination, bacteria filtration to biomolecule preconcentration. But these applications have been limited by the ability to control the length of the diffusion layer that is commonly indirectly prescribed by the fixed geometric and surface properties of a nanofluidic system. Here, we demonstrate that the depletion layer can be dynamically varied by inducing controlled electrothermal (ET) flow driven by the interaction of temperature gradients with the applied electric field [1]. To this end, a series of microscale heaters, which can be individually activated on

demand are embedded at the bottom of the microchannel and the relationship between their activation and ionic concentration is characterized. Moreover, in a different microfluidic setup that can support net flow we demonstrate that local ET stirring is efficient in controlling the location of the preconcentrated biomolecule plug. Thus, enabling to dynamically overlap the preconcentrated plug with surface immobilized molecular probes for enhanced detection sensitivity and binding kinetics. This ET-based electroconvective control of the depletion layer extends previously studied induced-charge electro-kinetics based control [2] which is limited to low conductivity solutions. It is hence expected that such electrokinetic-based spatio-temporal control of the diffusion layer will bring new functionalities to concentration-polarization based microscale applications.

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Electroconvective Instability on High Water-permeable Ion-selective Membrane

Authors

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Abstract

Electroconvective instability near ion-selective membrane has gained great attentions in ion concentration polarization (ICP) platform that induces significant concentration gradient at both sides of the membrane under a sufficiently strong dc electric field. This is because after a threshold voltage, the platform becomes electrokinetically unstable, which generates an interesting increase in ionic current called overlimiting current. This allows additional ion transport through the membrane and, thus, enhances the power efficiency in various applications such as fuel cells, electrodialysis, and preconcentration.

Many studies have recently reported experimental and theoretical results about the electroconvective instability, mainly focusing on the structure of ion-selective membrane. For example, Lammertink's group showed electroconvective ion transport through cation exchange membranes which had non-uniform geometry such as square-wave structures and Mani's group presented the effect of the repeatedly patterned ion-permeable and ion-impermeable membranes on the onset of electroconvective instability. However, there is lack of study considering a water-permeability of the membrane on electroconvective instability, while there are a number of practical situations where the membrane absorbs water at great extent such as swollen hydrogel or bufferless biomolecular preconcentrator. In this work, we suggest a micro/nanofluidic device incorporated with high water-permeable ion-selective membrane. A rigorous experimental and theoretical analysis of the water-permeable effect were conducted based on in situ visualization and a fully-coupled numerical simulation.

The micro/nanofluidic device was fabricated with cation selective membrane (CEM) having multiple microchannels perpendicular to the membrane so that the effect of extra permeable flow could be investigated by increasing the velocity or changing the direction. This device generated the vortices even before reaching overlimiting regime due to additional electroosmotic flows at the side of the multiple microchannels. In addition, when the electric field and the velocity of convective flow were identical (i.e. absorbing water), two types of vortices were observed, but only one type of vortices were observed in the opposite case (i.e. releasing water).

Numerical simulation based on Poisson-Nernst-Planck and Navier-Stokes equations showed similar flow characteristics. Furthermore, circulating flows were generated from one microchannel to the other microchannel under a low permeable condition, but the circulation was suppressed due to the strong convective flow as the permeable flow increased. Thus, the velocity of permeable flow could also affect the electroconvective instability. In addition, the circulations between water-paths increased as the number of the microchannels increased, which could affect the onset of the electroconvective instability. Also, the water-paths are able to have the ion-selectivity due to the

narrow distance between CEMs (surface conduction), so that the current density of this system would be divided by two regimes (convection current dominant and conduction current dominant) according to the distance. These results importantly implicated the understanding and design of ion-selective membrane, especially for enhancing the power consumption using membrane system having interconnecting channels.

Effect of pulsed electric field on electroconvection according to the relaxation time of convection

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Abstract

Perm-selective ion transport phenomena through nanoporous membrane have attracted significant attention in various engineering applications such as separation, detection, desalination and fuel cell. Among the phenomena, ion concentration polarization(ICP) has been extensively studied because the confined environment in a micro/nanofluidic platform provides a new physical insight by the direct visualization of electrokinetic fields. While conventional ICP platforms have utilized dc bias, the application of pulsed electric field(PEF) in ICP has gained notable attention because of their supportive merits such as lowering water splitting rate, mitigating fouling effect and enhancement of power efficiency. Among the characteristic properties generated by PEF, frequency dependency of current in 3 distinct regimes of ICP (i.e. Ohmic, limiting and overlimiting regime) have been studied but the physical mechanism of enhancement of average current density by PEF compared to dc bias was still unclear in overlimiting regime where electro-convective instability is dominant.

In this work, we simulated the electroconvection under the exertion of PEF using full consideration of Navier-stokes equations and Poisson-Nernst-Planck equations by COMSOL multiphysics. We assumed an ideal perm-selective

membrane in a periodic domain and PEF had 1/2 duty cycle with offset. Since convection relaxation time (inversely proportional to Schmidt number), which represent the required time to reach steady state of convection, was key role in our research, we investigated two separated regimes (i.e. Stokes regime and inertia regime) depending on the multiplication of frequency (f) and convection relaxation time (τ_{EC}). One can divide two regimes at $f\tau_{EC}=1$.

As a result, the ensemble average current density linearly increased in Stokes regime, while it has an optimum point in inertia regime as similar as the previously reported experimental work by Nikonenko done in electrodialysis cell. Furthermore, overlimiting conductance was also peaked at the same frequency. Considering total averaged velocity has an optimum point at $f\tau_{EC}=1$ (border of two regimes), the ensemble average current density was enhanced not only by the restoration of concentration due to remanent vortex, but also by the effect of nonlinearity of flow. We will verify this observation using experiments by changing the Schmidt number in a micro/nanofluidic platform.

Extending the Taylor-Aris dispersion model to electro-osmotically driven Hele-Shaw flows

Authors

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Abstract

We present an extension of the Taylor-Aris dispersion model to Hele-Shaw flows. The focus of this work lies on electro-osmotic flows (EOF) obtained using surfaces with patterned electro-osmotic mobility. Via the inhomogeneous electro-osmotic mobility, a flow pattern results that is a superposition of an EOF and a pressure-driven flow. The fluid flow model is based on a depth-averaged 2D approach [1]. The model accounts for different types of boundary conditions at the solid surface, including slip boundary conditions for superhydrophobic surfaces. Based on that, a Taylor-Aris type model for the effective dispersion

coefficient of a concentration tracer is derived. The core of the model is a dispersion tensor that varies as a function of position.

As an application of the model, we present the optimization of micromixing in a Hele-Shaw cell driven by EOF over superhydrophobic surfaces induced by gate electrodes. The mixing protocol is based on the well-known “blinking-vortex-principle” [2], utilizing two co-rotating vortices with non-overlapping vortex centers (see figure 1). By periodically turning each of the vortices on and off, the region around the center point between the two vortices experiences chaotic mixing. Finite-element-based simulations of the mixing process were conducted that utilize the dispersion model mentioned above. Based on the simulations, optimized micromixing configurations are identified. In addition to the simulations, we show experimental results obtained in a prototypic Hele-Shaw cell, demonstrating the ability to control the local flow field both temporally and spatially as well as the ability to enhance mixing significantly.

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Electroosmotic flow over superhydrophobic surfaces

Authors

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Abstract

We present the first experimental demonstration of electroosmotic flow (EOF) enhancement and flow patterning on a superhydrophobic surface using gate electrodes. We design the system such that the liquid wets the hydrophobic surface in a Cassie state, and use the gate electrodes to induce charge at the

liquid-air interface, i.e. we do not rely for the EOF on the native zeta potential of the surface. We characterize the EOF for a wide range of gate voltages, pH values, and surface geometries.

Our experimental setup consists of a Hele-Shaw cell with a hierarchical superhydrophobic surface as the bottom surface under which we place one or more gate electrodes. We generate a driving AC field parallel to the surface, while synchronously inducing charge at the liquid-air interface using the gate electrode. Consequently, we produce EOF solely on top of the electrode, leading to an internal pressure gradient driving the flow in the surrounding regions, forming a dipole flow as predicted by theory (figure attached). We are able to reverse the direction of the flow by creating a phase shift between the gate and the driving fields.

While the induced zeta potential is orders of magnitude smaller than the native zeta potential, the flow velocities are comparable to the native EOF. This demonstrates that the reduced hydrodynamic resistance of the surface promotes fluidic actuation with comparatively low stimuli. We believe that further reduction of the dielectric thickness would enable EOF velocities that are significantly higher than those achievable with a no-slip surface, opening the door to the creation of versatile, digitally adaptive microfluidic devices.

Optimizing Charge-Discharge Cycles in Nanoporous Supercapacitors

Authors

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Abstract

Nanoporous supercapacitors attract much attention as green energy storage devices with remarkable cyclability and high power and energy densities. However, their use in high frequency applications is limited by relatively slow charging processes, while accelerating charging without compromising the energy storage still remains a challenging task. Here, we study in detail the charging and discharging behaviour of nanoporous supercapacitors with narrow

pores, which provide exceptionally high capacitances and stored energy densities. We scrutinize the dynamic modes of charging, revealing, in particular, a transient formation of crowded and dilute ionic-liquid phases inside the pores, which leads to co-ion trapping and correspondingly slow charging. We show how trapping can be circumvented by applying a slow voltage sweep, and we demonstrate that it can accelerate the overall charging process considerably if the sweep rate is chosen appropriately. While one might be tempted to apply a similar strategy to discharging, we find that the best discharge rates are obtained when the voltage is switched off in a step-like fashion, whereby the optimal charge and discharge times differ few-fold. We unveil the scaling laws for such optimal quantities, which allow one to predict quantitatively the charging behaviour for realistically long pores. Based on our findings, we propose an optimal charge-discharge cycle and elaborate on optimization strategies.

Modeling the Current Modulation of dsDNA in Nanopores — from Mean-Field to Atomistic and Back

Authors

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Abstract

All-atom molecular dynamics (MD) simulations of double stranded DNA (dsDNA) translocating through a cylindrical nanopore by Kesselheim et al. in 2014 have revealed that ions close to the surface of the DNA experience an additional friction contribution when compared to their bulk value. This friction is a key ingredient in reproducing the 2006 experimentally observed current modifications by Smeets and coworkers. While these findings were already incorporated into a coarse-grained model by Weik et al. in 2016, we now present an extended mean-field model for solving the electrokinetic equations of a dsDNA confined to a structureless cylindrical pore. This is done by incorporating a suitably constructed friction term into the Nernst-Planck equation. Solving the modified electrokinetic equations using a finite element method, we demonstrate that this model is able to reproduce experimental and atomistic

MD results for dsDNA current modulations. The advantage of our model is that it allows a fast evaluation of new geometric arrangements of the DNA within the cylinder.

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Dynamic Flow Patterning with Localized Field Effect Electroosmosis

Authors

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Abstract

The ability to move fluids at the microscale is at the core of many scientific and technological advancements. Whereas two-phase flows can be controlled by acting on a fluid-fluid interface through a variety of physical mechanisms (e.g. electro-wetting, dielectrophoresis, thermocapillary, etc.), microscale control of continuous phases remains a significant challenge. It relies on fixed geometries and it is highly limited by the use of discrete channels and mechanical valves.

Here we present a novel mechanism that leverages localized field effect electroosmosis to create dynamic flow patterns, allowing fluid manipulation without the use of physical walls. We control a set of gate electrodes embedded in the floor of a fluidic chamber using an AC voltage in sync with an external electric field, creating non-uniform electroosmotic flow distributions. These give rise to a pressure field that drives the flow throughout the chamber.

We show that a disk-shaped gate electrode results in an electroosmotic flow dipole, consisting in a uniform flow above the electrode and dipole flow around it, with an intensity that can be tuned in real-time by controlling the gate AC amplitude. By superposing this basic flow unit, we generate a range of unique flow patterns, including quadrupoles, nested dipoles, regions of recirculating flow surrounded by quiescent fluid and volumes of complete stagnation within a moving fluid. We also demonstrated the interaction of multiple gate electrodes with an externally generated flow field, allowing spatial modulation of streamlines in real time.

At the conference I will present our latest (unpublished) experimental results demonstrating the creation of such flow patterns and illustrate their use for microscale fluid control and particle sorting. We believe that such flow control will help break the existing link between geometry and functionality, bringing new capabilities to microfluidic systems.

Does Current Monitoring work for Nanochannels with thick electrical double layers?

Authors

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Abstract

Surface zeta potential is one of the most fundamental parameters that determines electrokinetic flow in micro- and nanochannels. Accurately quantifying zeta potential is thus very important for understanding ion/molecule transport in micro- and nanofluidics, which has been widely used in a variety of applications including biomolecule separation and pre-concentration, label-free sensing, electrokinetic pumping and power generation, as well as nanofluidic diode/transistors. However, unlike particles in suspension whose zeta potential can be easily measured by optical methods, the confined spaces in micro- and nanochannel prevents direct measurement of zeta potential on the liquid-solid interface. One convenient method to indirectly measure zeta potential in such cases is the solution displacement method, also known as current monitoring (CM), in which the time-dependent change of electrical current in a channel, induced by electroosmotic flow, can be monitored and correlated with zeta potential.

Although this method has been extensively used to measure zeta potentials in microchannels, its validity for nanochannels has remained elusive due to non-negligible effects of relatively thick electrical double layer and the resulting hydrodynamic dispersion. In this work, we systematically investigated the validity of current monitoring in nanochannels via numerical simulation. We simulated the current monitoring process under different scenarios and compared the zeta potential “measured” by current monitoring with the actual value. The effects of nanochannel surface charge density and height, the solution ionic concentration and viscosity as well as the ion diffusivity were studied.

Our results show that the zeta potential measured by current monitoring deviates from the actual value when the EDL thickness increases. The deviation is found to be related to the ratio between the Debye screening length and the nanochannel confinement, reaching one when the ratio is approaching zero. We also found that the deviation is directly related to the Schmidt number, i.e. the ratio of kinematic viscosity and ion diffusivity. Our findings provide guidelines for

using current monitoring in nanochannels, which enables us to accurately characterize zeta potential in nanochannels and thus to better control electrokinetic flow for various nanofluidic applications.

Electrokinetic microflow of non-Newtonian solutions in polyelectrolyte brush-grafted channels

Authors

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Abstract

Micro/nanochannels grafted with the polyelectrolyte (PE), which is a charged polymer in aqueous medium, have shown great promise for applications such as ion-transport based sensing, selection, and current rectification [1,2]. In this study, we investigated the electrokinetic flow of PE solutions by extending our previous studies concerning electrokinetic Newtonian microfluidics [3,4]. The complete model framework has been developed to quantify the pressure-driven electrokinetic flow in rectangular microchannels with PE brushed wall, by including almost all relevant parameters. The PE brush layer can be represented as a fixed charge layer with the *Alexander-deGennes brush model*, where charge distribution nearby channel wall consists of mobile charge in the medium solution and fixed charge in the brush layer. Since both electrolyte ions and dispersed PEs are presented inside the channel, each ion concentration should be determined by multi-species ion dissociation. Our explicit model for coupled flow field is fully taking account of the shear-thinning behavior, electric body force as well as *Brinkman type hydrodynamic friction* inside the brush layer [5,6]. The *Poisson-Nernst-Planck equations* are numerically solved for electric field with ionic transport, which is well describing the *Donnan potential* [7] at the soft channel.

Note that the rheological constitutive model of *Carreau type* is adopted to describe electrolytic non-Newtonian solutions, such as anionic polyacrylic acid (PAA). This presentation reports the new results regarding the electric potential profile due to space charge and the retardation of flow velocity in terms of information of brushed PAA, concentration of dispersed PAA, and bulk pH conditions. The magnitude of Donnan potential shows several times higher than that of the surface potential in a bare channel, but it becomes lower with increasing PAA concentration. As the PAA concentration increases, the flow rate slows down according to increased viscosity, and even further slows down at higher pH due to the swelling of PAA. PAA-bushed channel is advantageous for possible enhancement of streaming potential/current, but which appears ineffective for PAA concentration above *ca.* 1,000 ppm. It can be concluded that electrokinetic transport of PEs in the soft channel becomes significant in a useful basis for channel design and potential applications to the microfluidics and nanofluidics.

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Fluctuating hydrodynamics of electrolytes at electroneutral scales

Authors

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Abstract

At mesoscopic scales electrolyte solutions are modeled by the fluctuating generalized Poisson-Nernst-Planck (PNP) equations, which we show can reproduce all of the predictions of the Debye-Hückel-Onsager theory for dilute multispecies electrolytes [A. Donev and A. L. Garcia and J.-P. Péraud and A. J. Nonaka and J. B. Bell, *Current Opinion in Electrochemistry*, 13:1-10, 2019]. However, at length and time scales larger than the Debye scales, electrolytes are effectively electroneutral, and the charged-fluid PNP equations become too stiff to solve numerically. Here we formulate the isothermal incompressible equations of fluctuating hydrodynamics for reactive multispecies mixtures involving charged species in the electroneutral limit, and design a numerical algorithm to solve these equations [to appear in Phys. Rev. E 2019, ArXiv:1809.08163]. We use the electroneutral algorithm to study a gravitational fingering instability, triggered by thermal fluctuations, at an interface where an acid and base react to neutralize each other. Our results demonstrate that, because the four ions diffuse with very different coefficients, one must treat each ion as an individual species, and cannot treat the acid, base, and salt as neutral species. This emphasizes the differences between electrodiffusion and classical Fickian diffusion, even at electroneutral scales.

Fabrication of Antifouling Electroconductive Thin Film Composite Membranes

Authors

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Abstract

Fouling of membranes is the most significant obstacle for the development energy and cost-efficient membrane processes. Development of electroconductive membranes (ECMs) can potentially provide an effective solution to

improve antifouling properties of membranes. The application of electrical potentials to the ECMs offers a promising improvement to existing membrane-based water treatment processes. Membrane surface charge is one of the influential factors that affect fouling at the initial stage of filtration through electrostatic interactions. By applying voltage to a conductive membrane, membrane's surface becomes more negative and it can effectively hinder the attachment of water contaminants, which are primarily negatively charged. As a result, membrane cleaning interval can be prolonged which reduces the operating cost of the membrane process. In this work, we fabricated a novel and mechanically robust electro-conductive membrane by pressure-assisted laminating of reduced Graphene Oxide-Polyaniline (rGO-PANI) suspension on commercial polyethersulfone (PES) support layer. Prior to fabrication, graphene oxide (GO) nanosheets were synthesized based on modified Hummers' method. Then, reduced GO (rGO) nanosheets were prepared by heating GO at 1000 °C. The reduction procedure removes functional groups, such as R-OH, R-O, ROOH and ROR, rendering rGO high electrical conductivity because of its none or low oxidation state. Results for rGO film showed an electrical conductivity of 102 S cm⁻¹. It was determined that rGO-PANI ECMs fabricated using sulfuric acid as the dopant showed the best transport, electrical, and stability characteristics, making them ideal for water treatment applications. In the next step, the surface morphology, chemical composition and permeation properties of the synthesized rGO-PANI membranes were characterized by field emission scanning electron microscopy (FESEM), attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy, zeta potential measurements, contact angle analysis, and filtration tests (pure water flux and rejection of organic matters). The utilization of the rGO-PANI material led to significant advantages, including: (1) increased surface hydrophilicity; and (2) greatly improved stability under anodic conditions. Fouling experiments conducted with organic foulant sodium alginate demonstrated the capacity of the rGO-PANI ECMs for in situ oxidative cleaning, with membrane flux restored to 80% of initial value under an applied potential of 2 V. In addition, a model organic compound (methylene blue) was electrochemically transformed at high efficiency (85%) in a single pass through the anodically charged ECM. rGO-PANI ECMs were found to have improved resistance to anodic oxidation, with little degradation observed

up to an anodic potential of 2 V under neutral pH conditions. Thus, these membrane materials are promising candidates for electro-conductive membrane materials suitable to participate in electro-oxidation reactions.

Effect of Specific ions on the Reduction of Interfacial Tension by Ionic Surfactants

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Abstract

Salinity affects oil recovery in surfactant flooding. While the role of salinity is complex, in this study we focus on a single mechanism: how salinity impacts the reduction in oil/water interfacial tension by surfactants. We develop a predictive molecular thermodynamic model to quantify the effect of individual monovalent ions (such as Na⁺, Cs⁺, Li⁺ and Cl⁻) on the reduction of interfacial tension (IFT). We apply the model to a simple system containing dodecane and water with ionic surfactants. In the thermodynamic model, we capture the adsorption of an ionic surfactant at the fluid/fluid interface using a surface equation of state, and we capture the counter-ion distribution profiles of dissolved salts near the interface using a modified Poisson-Boltzmann equation. This equation permits modeling of specific-ion effects by incorporating ionic dispersion interactions, which depend on the polarizabilities and sizes of ions. To test the model, we calculate the IFT of dodecane/water at different concentrations of NaCl and CsCl, and compare with experimental measurements using force tensiometry. Initial results from the model and experiments agree well, with both showing that specific ions (NaCl and CsCl), in addition to total salinity, impact the efficiency of the surfactant in reducing IFT.

Nanopore Electrokinetic Tweezer for single nanoparticle characterization/ manipulation.

Authors

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Abstract

Developing techniques that can characterize and manipulate individual micro/nanoscale objects in solutions are of paramount importance in a broad spectrum of applications whose implications range from basic research to personalized medical diagnostics. Although, the past decade has witnessed the emergence of diverse powerful optical tools that can selectively detect and manipulate single micro-sized objects, it still remains a great challenge to integrate such techniques with lab-on-a-chip applications and more importantly to extend their capabilities for manipulating and characterizing nanosized objects. Here we present a novel electrokinetic tweezer for single nanoparticle manipulation and characterization based on electrokinetic trapping near a silicon nitride nanopore. We find that this nanopore-based electrokinetic tweezer simultaneously share lots of similarities with resistive pulse sensors and optical tweezers. We prove that nanoparticle trapping occurs due to a balance between electrostatic and hydrodynamic forces induced on the particle and that the motion of a trapped particle can be modeled as a harmonic oscillator, with the spring constant of the system being the trap stiffness. We show that different values of ionic currents through the nanopore and trap stiffnesses are achieved when trapping nanoparticles with different sizes (down to 100 nm) and/or surface charge densities. We also demonstrate that the nanoparticle trap stiffness and position can be controlled with a force resolution of the order of pN, and position resolution of nm, by tuning the applied voltage and buffer

concentration. The technique we have uncovered could potentially be harnessed in novel micro-nanofluidic applications such as in lab-on-a-chip devices, transport control and nanophotonics.

From Electrodifusion Theory to the Electrohydrodynamics of Leaky Dielectrics through the Weak Electrolyte Limit

Authors

Prof. Yoichiro Mori - University of Minnesota

Dr. Yuan Young - New Jersey Institute of Technology

Abstract

The Taylor-Melcher (TM) model is the standard model for describing the dynamics of poorly conducting leaky dielectric fluids under an electric field. The TM model treats the fluids as Ohmic conductors, without modeling ionic electrodiffusion. Mathematical reconciliation of the electrodiffusion picture and the TM model has been a major issue for electrohydrodynamic theory. Here, we derive the TM model from an electrodiffusion model the electrochemistry of ion dissociation is modeled explicitly. We introduce salt dissociation reaction terms in the bulk electrodiffusion equations and take the limit in which the salt dissociation is weak (i.e., poorly conducting media). Together with the assumption of small Debye length, we derive the TM model with the surface charge convection term. An important quantity that emerges is the Galvani potential (GP), the jump in voltage across the liquid-liquid interface between the two leaky dielectric media. When the GP is absent, we recover the TM model. In the presence of a non-zero GP, our model predicts that the liquid droplet will drift under an imposed electric field, the velocity of which is computed explicitly to leading order.

References: Y. Mori and Y.N. Young, *From Electrodifusion Theory to the Electrohydrodynamics of Leaky Dielectrics through the Weak Electrolyte Limit* Journal of Fluid Mechanics 855, 67-130 2018

Theory of freezing point depression and freeze-thaw damage by nano-fluidic salt trapping

Authors

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Abstract

A remarkable variety of wet porous materials and life forms are able to endure temperatures far below the freezing point of bulk water, where others are fatally damaged. Freeze-thaw survival in biology is usually attributed to “anti-freeze” solutes, and yet in many durable materials, only aqueous electrolytes are present in the pores. For concrete pavements, freeze-thaw damage is believed to result from the expansion of water upon freezing, which can be inhibited by de-icing salts (lowering the bulk melting point) or confinement in nanopores (Gibbs-Thompson effect). This belief contradicts the observed correlation between damage and de-icing salts, and freezing damage of benzene loaded cement paste. None of these mechanisms can explain the freezing pressures (up to 10 MPa) or supercooling (down to -40 C).

In this letter, we propose an alternate hypothesis – nanofluidic salt trapping – which is able to rationalize experimental observations, using simple mathematical models of dissolved ions trapped in thin liquid films between growing ice and charged surfaces. The theory predicts that large disjoining pressures can be generated, and ice nucleation suppressed, until salt precipitation or neutralization of the surface charge allows complete freezing and release of the pressure.

Flow-Induced Surface Charge Heterogeneity in Electrokinetics due to Stern-Layer Conductance Coupled to Reaction Kinetics

Authors

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Mr. Ben Werkhoven - Utrecht University

Dr. Jeffrey Everts - University of Ljubljana

Abstract

We theoretically study the electrokinetic problem of a pressure-induced liquid flow through a narrow long channel with charged walls, going beyond the classical Helmholtz-Smolukowski picture by considering the surprisingly strong combined effect of (i) Stern-layer conductance and (ii) dynamic charge-regulating, i.e. the surface charge is laterally mobile rather than fixed and can adsorb-desorb in directions normal to the wall surface. We will see that the pressure-induced water flow induces, apart from the well-known streaming potential, also a strongly heterogeneous surface charge and zeta potential on chemically homogeneous channel walls. Moreover, we identify a novel steady state with a nontrivial 3D electric flux with 2D surface charges acting as sources and sinks. For a pulsed pressure drop our findings also provide a first-principles explanation for ill-understood experiments on the effect of flow on interfacial chemistry [D. Lis *et al.*, *Science* **344**, 1138 (2014)]. We will support our numerical calculations with analytic results. If time permits, we will show recent results on diffusio-osmotic and diffusio-electric transport.

Our findings were published in

Flow-Induced Surface Charge Heterogeneity in Electrokinetics due to Stern-Layer Conductance Coupled to Reaction Kinetics, B. L. Werkhoven, J. C. Everts, S. Samin, and R. van Roij, *Phys. Rev. Lett.* **120**, 264502 (2018).

Dynamic Stern layers in charge-regulating electrokinetic systems: three regimes from an analytical approach, B. Werkhoven, S. Samin, and R. van Roij, Eur. Phys. J. Special Topics (2019); arXiv:1809.03287.

Polarization processes at the electrical treatment of dispersed systems

Authors

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Abstract

The electric field is widely used in the processing of dispersed systems (dehydration and decontamination of concentrated dispersions from impurities, electrocoagulation of particles and droplets in dilute dispersions, etc.). One of the important scientific and practical problems is the electrical decontamination of fine clay slurries and soils from charged (heavy metals, radionuclides) and uncharged (hydrophobic organic substances) impurities).

Application of an electric field causes several mechanisms of impurities transfer, such as electromigration, electrophoresis, electroosmosis. However, the efficacy of these mechanisms is substantially limited by accompanying chemical and electrochemical processes, the features of which depend both on the nature of treated dispersions and on the conditions of developed processes.

The used methods of soil electroremediation are accompanied by water electrolysis on electrodes leading to the transport of H and OH ions into soils,

which usually plays negative role changing local distribution of electric field, local electrokinetic potential of soil particles and velocity of electroosmosis, solubility and mobility of impurities. From another side, the electrolysis can play the positive role, since the electrodes as sources of H and OH ions can be used for directed pH regulation of materials under treatment. The proposed by us method of electrohydrodynamic regulation of soil pH allowed to reach the desirable low or high value of soil pH and to increase the efficacy of soil decontamination.

The distribution of electric field in soil and the peculiarities of its remediation are investigated experimentally using kaolinite contaminated with either heavy metals (Cu, Cd) or organic hydrophobic pollutants (chlorobenzene, orthochlorotoluene, cyclohexilbenzene) as a model systems. The obtained experimental data strongly depend on the polarization processes in the system, which in turn depend on voltage and the electrolyte solutions used in the electrode chambers and wetting the soil.

To optimize the electroremediation the theoretical model describing electromigration processes, the change of voltage, pH distribution and related electrokinetic potential and electroosmosis in the soil was developed. The features of these changes in the galvanostatic and potentiostatic modes with a different ratio of electromigration mobilities of cations and anions in the soil and that of a substituting ions coming from the electrodes chamber were considered.

The performed theoretical analysis within the framework of a simplified three-ions model made it possible to reveal differences between the galvanostatic and potentiostatic modes and set main qualitative regularities of the processes being studied. The developed model is applicable for soils with a low exchange and buffer capacities, when the substituting ions coming from the anode chamber are spent only on supplanting mobile ions, but are not used for ion exchange and chemical reactions.

A semi-quantitative theoretical estimate of reducing the speed of movement of supplanting mobile ions and the rate of soil decontamination caused by exchange and buffer capacities of the soil was performed.

Despite substantial simplifications in the developed model, the numerical analysis sufficiently well agrees with the experimental data for decontamination of the soil from heavy metals and organic hydrophobic impurities.

Optimized Coagulation Pathway of Al₁₃: Effect of In-situ Aggregation of Al₁₃

Authors

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Abstract

Particle coagulation by Al₁₃ has been extensively investigated for drinking water and waste water treatment, the well-accepted mechanisms including charge neutralization and electrostatic patch were proposed to dominate coagulation reactions. However, the detailed pathways of particle coagulation including the interactions between Al₁₃ and particles, particles and particles, and also the evolution of Al₁₃, remain unclear. Since Al₁₃agg (Al₁₃ aggregate) was found in flocs, the real coagulation process should be different from previous understanding. In this study, to make clear the details of aggregation of Al₁₃ and its effect on coagulation performance, we designed two coagulation tests for silica suspensions by preformed Al₁₃agg and Al₁₃, respectively. The results showed that optimized coagulation for particle removal by Al₁₃ occurred under neutral and alkaline conditions, which was dominated by in-situ aggregation of Al₁₃. The results of ²⁷Al-NMR and XPS confirmed that Al₁₃agg existed in both flocs, but the differences in Al distribution and morphology between two tests have been observed via SEM and EDS. The in-situ formed Al₁₃agg covered all over the particles, resulting in compact flocs with a rough surface. In contrast, the preformed Al₁₃agg mainly distributed on joint sites between particles,

generating denser and glossy flocs. This difference verified that in-situ aggregation of Al_{13} was the key factor for optimized particle coagulation. Overall coagulation for efficient particle removal by Al_{13} should undergo charge neutralization-in-situ aggregation of Al_{13} -interparticle bridging processes. Aggregation of Al_{13} readily occurred at high pH, thus efficient particle removal could be achieved in neutral and alkaline waters.

Autonomous NanoSurfactant for Enhanced Oil Recovery Applications

Authors

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Abstract

Enhanced oil recovery (EOR) techniques often involve delivering chemicals, macromolecules, or particles in oil reservoirs to improve oil mobility and production. The harsh environment typical to the reservoir poses a great challenge to maintaining long-term stability of these agents. Moreover, accessing constricted regions in the reservoir with extremely tight pores and pore throats, and where large volumes of resources exist, require more efficient delivery methods than diffusion.

We have developed an in-house EOR nano-agent (NanoSurfactant) platform using the inexpensive and abundant petroleum sulfonate salt surfactant. NanoSurfactants are chemically and colloidally stable at high salinity (> 56k ppm) and high temperature (> 90 °C) conditions. The structure, size, and surface properties of NanoSurfactants suggest different transport mechanisms for enhanced delivery in oil reservoirs compared to conventional surfactants. We seek to improve the delivery of NanoSurfactants to regions in the reservoir that are inaccessible to conventional waterflood. Here, we explore diffusiophoresis as a means to efficiently deliver NanoSurfactants to flow-restricted regions.

Experiments are conducted to directly observe the diffusiophoretic migration of NanoSurfactants in different chemical gradients. These transient gradients are established in microfluidic channels mimicking dead-end pores in the reservoir. In addition, we study the effect of adding dilute macromolecules to the NanoSurfactant solutions on their diffusiophoretic migration. NanoSurfactants are labelled with a fluorescent dye to enable microscopic visualization and quantification of diffusiophoretic migration.

Results showed that salinity gradients yield faster and deeper delivery of NanoSurfactants into the dead-end channels compared to diffusion without any gradients. More pronounced migration is observed when small concentrations of macromolecules are added.

Our findings expand the understanding of diffusiophoretic migration in extremely high salinity environment. Also, they provide insights into the utilization of natural or induced gradients in oil reservoirs to harness the diffusiophoretic migration for EOR applications.

Hydrodynamic and electrokinetic transport of liquid and microparticles in porous materials

Authors

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Abstract

One of the most common methods of water decontamination of dispersed pollutants is mechanical filtration either through filters filled by sand, clay, ions exchangers or through porous diaphragms. The filtration using the pressure only is often not sufficiently effective, but can be enhanced by an electric field.

When the filter is filled by the grains (the particles of material-collector) the delivery of charged pollutants to the grain surface at electrical field is ensured not only by their hydrodynamic transport, but also by their electrophoresis and electroosmosis along the grain surfaces. In addition, the polarization of the collector grains creates the conditions for diffusiophoresis and dipolophoresis.

Theoretical investigation of the mechanism of interaction of dispersed pollutants and the grains for effective control of the electrofiltration is carried out. The non-uniform electric field in the gaps between the grains and the transport to their surface of charged pollutants substantially depend on the relationship between the electric conductivities of the grains and the solution affecting both the distribution of the field in the gap and polarization of the grains and pollutants, which affects the electrofiltration efficiency.

Microscopic study of the sediment of dispersed particles, bacteria and micromycetes on the grains made it possible to draw a conclusion about its structure and the formation mechanism. It was found that the sediment is chains of many particles long separated by intervals, which are formed thanks to dipole interaction of pollutants with the grains and between themselves. It was also established that the sediment thanks to its loose structure after switching off the electric field is easily washed away by a small amount of water.

Charged porous diaphragms are used both for filtration and for separating the anodic and cathodic zones when conducting electrochemical water disinfection. In the latter case, water filtration through a porous diaphragm is combined with simultaneous production of active chlorine at the anode.

Although the diameter of the cylindrical pores is noticeably larger than the bacteria size, over time the filtration becomes deteriorated due to fouling caused by bacteria accumulation. Since the disinfecting effect of the electric field does not depend on its direction, studies of the efficiency of such a filter during polarity reversal were carried out.

With the simultaneous action of pressure and electric field, a complex profile of the bacteria velocity over the pore cross-section arises. In the center of the pores the bacteria velocity is mainly determined by the liquid flow, and in the

near-wall it is determined by the sum of the speeds of electroosmosis and electrophoresis.

Thus, depending on the location of the cathode and the anode, as well as the electrokinetic potentials of the pore walls and bacteria, the latter move either in the direction of the hydrodynamic flow or against it.

An increase in filter efficacy occurs when electroosmosis is directed in the opposite way to the hydrodynamic flow, which leads to local water turbulization in the near-wall area and, consequently, worsens bacteria adhesion to the wall, which prevents clogging of the pores.

Induced Charge Electroosmotic Flow Including Finite Ion Size Effects

Authors

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Abstract

We present a numerical simulation approach on geometrically flexible unstructured meshes which combines a pressure-robust, mixed finite element method for the Stokes equations admitting an divergence-free postprocessing with optimal complexity [1] with a thermodynamically consistent finite volume method for the discretization of ion drift and diffusion in a self-consistent electric field based on a generalized Nernst-Planck-Poisson system which takes into account finite ion size and solvation effects [2,3].

Using this method, we investigate direct current induced charge electro-osmotic flow phenomena at nanoscale electrodes [4]. In particular, we study the interaction between convective and diffusive transport of reaction intermediates between two flat coplanar nanoelectrodes with different potential.

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Effect of the double layer structure on the photo-induced charge transfer across the interface between two immiscible liquids

Authors

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Dr. Micheal Scanlon - University of Limerick

Abstract

Photo-induced charge transfer across interfaces is a fascinating process that has yet to be fully understood at the molecular level.[1] Significant progress has been made in understanding photo-induced electron transfer across solid-solid or solid-liquid interfaces, which ultimately will have a big impact on the performance of technologies related to solar energy conversion and storage.[2] However, charge transfer across membrane-like interfaces, like the interface between two immiscible liquids, remains rather unexplored.[3], [4]

In this presentation, we will share our work exploring the photo-induced charge transfer phenomena at the interface between water and a highly hydrophobic organic solvent like trifluorotoluene. To do this, we will present results obtained

using a simple system where the interface between these two immiscible liquids is functionalized with a nanostructured film of zinc tetrakis(4-carboxyphenyl) porphyrin or ZnTPPc . Once the interface was functionalized, we studied the effect of a potential difference between the two liquids (Galvani potential difference) on the photo-induced electron transfer between ferrocene derivatives in the organic solvent and oxygen in water, using photocurrent spectroscopy. Depending on the structure of the interface and on the potential of zero charge, three potential regions with different photo-response were observed: region I or photo-capacitance region, region II in which cations are the main charge carriers across the interface and region III where electrons are. Control of the Galvani potential difference and the chemical nature of the ferrocenes, allows the transfer of one of the carriers to be favored. "Band bending" effects and the presence of a Schottky-type barrier at the interface were also observed and will be discussed.

Keywords: Porphyrins, Galvani potential difference, Photocurrents, Photo-induced charge transfer

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Role of Stefan-Maxwell fluxes in the dynamics of concentrated electrolytes

Authors

Ms. Bhavya Balu - Carnegie Mellon University

Prof. Aditya Khair - Carnegie Mellon University

Abstract

This theoretical analysis investigates the effect of ambi-polar diffusion and coupled ionic fluxes on the dynamics of the charging of an electrochemical cell. We consider a model cell consisting of a concentrated, binary electrolyte between parallel, blocking electrodes, under a suddenly applied DC voltage. It is assumed that the applied voltage is small compared to the thermal voltage, $\$R T/F\$, where $\$R\$$ is the universal gas constant, $\$T\$$ is the temperature and $\$F\$$ is the Faraday's constant. We employ the Stefan-Maxwell equations to describe the hydrodynamic coupling of ionic fluxes that arise in concentrated electrolytes. These equations inherently account for asymmetry in the mobilities of the ions in the electrolyte. A modified set of linearized Poisson-Nernst-Planck equations, obtained by incorporating Stefan-Maxwell fluxes into the species balances, are formulated and solved analytically. A long-time asymptotic analysis reveals that the electrolyte dynamics occur on two separate time scales. A faster, RC time, $\tau_{RC} \sim \kappa^{-1} L / \mathcal{D}_E$, where \mathcal{D}_E is an effective diffusivity, characterizes the evolution of charge density at the electrode. The effective diffusivity, \mathcal{D}_E , is a function of the ambi-polar diffusivity of the salt, \mathcal{D}_a , as well as a cross-diffusivity, \mathcal{D}_{+-} , of the ions. This time scale also dictates the initial exponential decay of current in the external circuit. At times longer than τ_{RC} , the external current decays exponentially with a slower, diffusive time scale, $\tau_D \sim L^2 / \mathcal{D}_a$, where, \mathcal{D}_a is the ambi-polar diffusivity of the salt. This diffusive time scale is due to the unequal ion mobilities that result in a non-uniform bulk concentration of the salt during the charging process.$

Ion adsorption, hydration, and the structure of the electric double layer: classical ideas and recent insights from high resolution Atomic Force Microscopy

Authors

Prof. Frieder Mugele - University of Twente

Abstract

Surface charge and the distribution of ions in the vicinity of solid-water interfaces play a central role in colloid science and are thereby essential for a wide range of phenomena and processes in nature, science, and technology. Theoretical models of the solid-electrolyte interface date back to the late 19th and early 20th century. Prof. Hans Lyklema (1930-2017) devoted much of his scientific life to the investigation and deeper understanding of this interface at the interface between physics and chemistry. Throughout most of his career, experimental techniques to characterize electric double layers relied on macroscopic averaging and therefore lacked the spatial resolution to directly test many of the ideas that he and others proposed. In recent years, advances in x-ray surface diffraction and absorption spectroscopy, non-linear optics, and high-resolution Atomic Force Microscopy (AFM) along with improved numerical simulations tools have enabled a deeper look into the arrangement of ions and solvent molecules at this interface. In this lecture, I will highlight some of the key lessons learned from these novel techniques, focusing largely on results from in situ AFM studies, and I will comment on some consequences of these results for macroscopic phenomena. Given the growing need for efficient and reliable (electro)chemical conversion and energy storage technologies, these insights will be essential in addressing some of the most severe challenges that modern societies are facing.

Theory of coupled ion transport and chemical conversions in bioelectrochemical systems

Authors

Mr. Aymar de Lichtervelde - Wageningen University

Dr. Maarten Biesheuvel - Wetsus

Dr. Hubertus V. M. Hamelers - Wetsus

Dr. Annemiek ter Heijne - Wageningen University

Dr. Jouke Dykstra - Wageningen University

Abstract

Bioelectrochemical systems are electrochemical cells that rely on a conductive biofilm covering an electrode. Such biofilm is analogous to a membrane, excepted that it is also reactive and electrically conductive. Considering the example of a microbial fuel cell, we derive a dynamical model of ion transport, biochemical reactions and electron transport inside such a biofilm. After validating the model against experimental data, we evaluate model output to obtain an understanding of transport of ions and electrons through a current-producing biofilm. For a system fed with a typical wastewater stream containing organic molecules and producing 5 A m², our model predicts that transport of the organic material is not a limiting factor. However, the pH deep inside the biofilm drops significantly, which can inhibit current production of such biofilm. Our results suggest that experimentally-obtained electrical conductivities do not limit charge transport significantly, even for a biofilm of 100 micrometers in thickness. Our study provides an example of how physics-based modelling helps to understand complex coupled processes in bioelectrochemical systems.

Sculpting Diffusiophoretic Migration with Reactive Solutes

Authors

Dr. Xiaoyu Tang - University of California, Santa Barbara

Dr. Nan Shi - Saudi Aramco

Mr. Anirudha Banerjee - University of California, Santa Barbara

Dr. Amr Abdel-Fattah - Saudi Aramco

Dr. Afnan Mashat - Saudi Aramco

Prof. Todd Squires - University of California, Santa Barbara

Abstract

Particle delivery/extraction in dead-end pores is critical in many applications such as drug delivery and oil recovery. Due to geometrical confinement, convective flow is suppressed. Particle diffusion is the most accessible mechanism but is prohibitively slow. One promising strategy to deliver particles in dead-end pores is diffusiophoresis, in which solute concentration gradient drives particle migration. The solute concentration gradient is commonly imposed by introducing a solution of higher or lower concentration and relying on solute diffusion to generate the gradient. However, since the diffusiophoretic velocity does not depend on the imposed solute concentration, single solute offers very little control. Here, we present a new and versatile strategy to create solute gradient to drive diffusiophoretic particle migration: chemical reaction generated solute gradient. We will demonstrate that the speed and concentration of the particles can be controlled by varying particle diffusiophoretic mobility, reactant concentration ratio, and reactant diffusivity ratio. Different particle delivery pattern can be achieved: non-focusing or focusing where particles are delivered in a concentrated band. A theoretical model that directly predicts the particle migration dynamics agree well with the experiment. Diffusiophoresis under reactive solute gradient opens up new possibilities to manipulate particle migration in many configurations and applications.

Diffusiophoretic migration of colloids induced by freely falling soluto-inertial beacons

Authors

Mr. Anirudha Banerjee - University of California, Santa Barbara

Prof. Todd Squires - University of California, Santa Barbara

Abstract

The range of equilibrium colloidal interactions in aqueous suspensions is limited to less than a micron. We recently demonstrated a novel concept that can be used to drive non-equilibrium suspension interactions over millimeter length scales using chemical “beacons” that establish and maintain solute gradients (or chemical potential gradients) in-situ. These gradients drive diffusiophoretic migration of suspended particles, the direction of which is sensitive to the specific interaction between the out-fluxing solute from the beacon and the surface of the particles. Previous experimental work was restricted to fixed, cylindrical beacon structures to visualize and study the general scope of these so-called “solute-inertial” (SI) interactions under a controlled, microfluidic environment. We now move on to a broader application of this phenomenon by showing that free falling, 3-dimensional beacon “particles” can be used to generate solute gradients in bulk suspensions and thereby attract (or repel) colloids to (from) specific locations in the suspension. As the beacon falls down, it leaves a solute wake behind it, which then diffuses radially outwards to establish the concentration gradient required to drive SI colloidal migration. Theoretical predictions and experimental observations capture the scope of these interactions in terms of the size and falling speed of the beacon particles and their ability to collect suspended objects. With this basic understanding, we believe that we can further extend the framework to design freely suspended “colloidal beacons” that will not only establish gradients but also migrate in response, potentially creating new possibilities in the field of active matter and self-assembly.

Electrokinetic flows on nanostructured superhydrophobic surfaces

Authors

Mr. aktaruzzaman al hossain - Stony Brook University

Dr. Antonio Checco - Stony Brook University

Dr. Carlos Colosqui - Stony Brook University

Abstract

The flow of electrolyte solutions confined by nanostructured superhydrophobic surfaces can enable micro/nanofluidic devices for conversion of hydrostatic pressure into electrical current with high efficiencies. Experimental measurements and molecular dynamics simulations performed by our group confirm that unexpectedly large zeta potentials can be attained on nanostructured superhydrophobic surfaces with small geometric features on the order of the Debye length. Experimental measurements for conventional and nanostructured silica surfaces coated with octadecyltrichlorosilane (OTS) report slip lengths of 30--40 nm and zeta potentials well in excess of 50 mV. The measured zeta potentials are sensitive to variations in the electrolyte concentration, the solution pH, and type of electrolyte employed (e.g., KCl or NaCl). Analytical predictions from the Poisson-Boltzmann and Navier Stokes equations considering the presence of hydrodynamic slip and hydration forces are employed to interpret experimental observations and to account for results from molecular dynamics simulations. Analytical predictions indicate that the employed surfaces can enable mechanical-to- electrical power conversion efficiencies larger than 30% when electrolyte solutions flow in nanoscale slit channels with heights on the order of 100 nm.

Continuous Diffusiophoretic Nanoparticle Separation by Enhanced Ion Exchange

Authors

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Prof. Sung Jae Kim - Seoul National University

Prof. Hyomin Lee - Jeju National University

Mr. Sungmin Park - Seoul National University

Mr. Dokeun Lee - Seoul National University

Abstract

Nanoparticles have been widely utilized for the state-of-the-art healthcare platform, point-of-care and purification due to their versatile functionalities. Thus, an effective and efficient separation of the nanoparticles have been highly demanded recently. Comparing to conventional batch-type method (e.g. filtration, chromatography and centrifugation), micro/nanofluidic platform has provided continuous separation strategies. For example, ion concentration polarization phenomenon or an inertial microfluidic device utilizing Dean-coupled inertial migration have been successfully demonstrated for the nanoparticle separation. However, these methods required high voltage, complicated fabrication or extremely long separation channel. Here, in this work, we present a new approach to continuously separate nanoparticles based on diffusiophoresis which is a particle migration mechanism induced by a concentration gradient without the external stimuli such as electric field, magnetic field, or acoustic waves. Especially, the concentration gradient is generated by ion exchange phenomenon near a cation-exchange membrane due to the diffusivity difference between cations of buffer solution and protons in the membrane, resulting in the spontaneous development of the concentration gradient in the vicinity to the membrane. Moreover, we demonstrated enhancing the separation efficiency by adjusting the pH of neighboring electrolyte solution.

To fabricate micro/nanofluidic ion exchange platform, Nafion was used as a cation-exchange membrane. The Nafion membrane was patterned parallel to the direction of buffer and sample streams to induce 1:1 exchange of dissolved cation (Na^+) and inner proton (H^+) of the membrane. The diffusiophoretic force which was induced by concentration gradient repelled the colloidal suspension, leading to the exclusion layer (*i.e.* particle-free layer) along the direction of streams. Due to the different diffusiophoretic mobility of nano-colloidal suspensions consisted of 40 nm, 200 nm and 2,000 nm particles, each suspension possessed distinguishable exclusion distance so that the continuous separation was achieved without external electric field. Furthermore, as Tris or NaHCO_3 buffer solution was injected, the reaction of buffer solution having exchanged protons and the solution (Tris or NaHCO_3) increased the

concentration gradient by removing protons in the buffer stream. Enhanced diffusiophoretic migration due to the increased concentration gradient can provide a higher separation resolution. Also, we controlled the exclusion distance by changing the concentration of the injected buffer solution. These results implied that the nanoparticle separation was successfully accomplished only by the salt gradient-induced force and our separation method would provide an economic approach for detection of fine dusts, point-of-care system or pharmaceutical products.

Zeta potential of the mineral-brine interface in natural, intact carbonates: implications for improved oil recovery by controlled salinity waterflooding.

Authors

Prof. Matthew Jackson - Imperial College London

Mr. Harry Collini - Imperial College London

Abstract

Despite the broad range of interest and applications, controls on the zeta potential in natural carbonates remain poorly understood. The zeta potential is an important measure of the electrical potential at the mineral surface, and the magnitude and sign of the zeta potential control the electrostatic interactions between the mineral surface and polar species in aqueous and non-aqueous solution. Natural systems typically host brines of high ionic strength containing a wide range of salt species, at elevated temperature compared to typical laboratory conditions and, in oil reservoir rocks, also host crude oil that can change the wetting behaviour of the mineral surfaces. Measuring the zeta potential at conditions relevant to such systems is challenging.

Here we report measurements of the zeta potential in a range of different intact natural carbonate samples, equilibrated with brines of varying composition and ionic strength, and crude oils of varying composition, over the temperature range relevant to oil reservoirs. Zeta potential was measured using the streaming potential method implemented in a bespoke, in-house experimental

setup. The method is applicable to intact natural rock samples, can be used to measure zeta potential at high ionic strength, elevated temperature and pressure, using samples saturated with more than one fluid phase.

Our results confirm that the zeta potential responds to the concentration of key divalent ions Ca, Mg, CO₃ and also possibly to SO₄. pH is directly correlated to the concentration of Ca and Mg, yielding an apparent relationship between zeta potential and pH. Reducing the ionic strength and changing the composition from typical oil reservoir brines to seawater and then dilute seawater tends to switch the zeta potential from positive to increasingly negative owing to the decreased concentration of Ca, with Mg and SO₄ playing a more minor role. The same trend pertains, irrespective of temperature, over the range typical of oil reservoirs.

It is well known that modifying the injection brine composition during waterflooding by controlling the type of ionic species present or the total ionic strength can lead to improved oil recovery (IOR). Moreover, previous work has suggested that IOR can be correlated with changes in zeta potential at the mineral-brine and oil-brine interfaces in carbonates.

Here we report a large new suite of carbonate zeta potential data and coreflood results. These demonstrate that the zeta potential at both the mineral-water and oil-water interfaces must be determined when designing the optimum brine composition for CSW. We conclude improved recovery during CSW is observed only if the change in brine composition yields a zeta potential at each interface that has the same polarity, such that a repulsive electrostatic force acts between the interfaces and stabilizes a water film on the mineral surface.

Understanding Calcium-Mediated Adhesion of Nanomaterials in Reservoir Fluids: Insights from Molecular Dynamics Simulations

Authors

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Dr. Shannon Eichmann - Aramco Services Company: Aramco Research Center-Houston

Prof. Nancy Burnham - Physics and Biomedical Engineering Departments, Worcester Polytechnic Institute

Abstract

Interest in nanomaterials for subsurface applications has grown markedly due to their successful application in a variety of disciplines, such as biotechnology and medicine. Nevertheless, nanotechnology application in the petroleum industry presents greater challenges to implementation because of the harsh conditions (i.e. high temperature, high pressure, and high salinity) that exist in the subsurface that far exceed those present in biological applications. The most common subsurface nanomaterial failures include colloidal instability (aggregation) and sticking to mineral surfaces (irreversible retention). A previous atomic force microscopy (AFM) study demonstrated that carboxylate alkanethiol functionalized AFM tips showed mitigated adhesion forces in calcium ion rich fluids. Herein, molecular dynamics simulations reveal the molecular-level details in the AFM experiments. The simulation results unambiguously showed that in calcium ion rich fluids, the strong carboxylate-calcium ion complexes prevented direct carboxylate-calcite interactions, thus lowering the AFM adhesion forces. We performed the force measurement simulations on five representative calcite crystallographic surfaces and observed that the adhesion forces were about two to three fold higher in the calcium ion deficient fluids compared to the calcium ion rich fluids for all calcite surfaces. Moreover, in calcium ion deficient fluids, the adhesion forces were significantly stronger on the calcite surfaces with higher calcium ion exposure. This indicated that the interactions between the functionalized AFM tips and the calcite surfaces were mainly through carboxylate interactions with the calcium ions on calcite surfaces. Finally, when analyzing the order parameters of the tethered functional groups, we observed significantly different behavior of the alkanethiols depending on the absence or presence of calcium ions. These observations agreed well with prior AFM experiments and provided new insights for the competing carboxylate/calcite/calcium ion interactions.

Zeta potential of the mineral-brine interface in natural, intact sandstones with oilfield applications

Authors

Mr. Harry Collini - Imperial College London

Prof. Matthew Jackson - Imperial College London

Abstract

The zeta potential is an important measure of the electrical potential at the mineral surface, and the magnitude and sign of the zeta potential control the electrostatic interactions between the mineral surface and polar species in aqueous and non-aqueous solution. Natural systems typically host brines of high ionic strength containing a wide range of salt species, at elevated temperature compared to typical laboratory conditions and, in oil reservoir rocks, also host crude oil that can change the wetting behaviour of the mineral surfaces. Measuring the zeta potential at conditions relevant to such systems is challenging.

Here we report measurements of the zeta potential in a range of different intact natural sandstone samples, equilibrated with brines of varying composition and ionic strength, and crude oils of varying composition, over the temperature range relevant to oil reservoirs. Zeta potential was measured using the streaming potential method implemented in a bespoke, in-house experimental setup. The method is applicable to intact natural rock samples, can be used to measure zeta potential at high ionic strength, elevated temperature and pressure, using samples saturated with more than one fluid phase.

It is widely accepted that the zeta potential in sandstones is negatively charged and increases in magnitude with decreasing ionic strength for indifferent ions. However, little data are available regarding the zeta potential in sandstones saturated with complex brines typical of those present in oil reservoirs at reservoir conditions. Our results show that zeta potential for a given complex brine can vary significantly depending upon the specific minerals present in the

sandstone. In some samples, decreasing ionic strength may yield no change, or a more positive zeta potential, contrary to the general assumption.

It is well known that modifying the injection brine composition during waterflooding by controlling the type of ionic species present or the total ionic strength can lead to improved oil recovery (IOR). Moreover, previous work has suggested that IOR can be correlated with changes in zeta potential at the mineral-brine and oil-brine interfaces, if the change in brine composition yields a zeta potential at each interface that has the same polarity, such that a repulsive electrostatic force acts between the interfaces.

Here we report zeta potential data and coreflood results made on sandstones with varying clay content. Clay minerals have been argued to be an important factor in controlled salinity waterflooding in sandstones. We discuss the impact of these on our results and examine the correlation between IOR and changes in zeta potential at the mineral-brine and oil-brine interfaces in sandstones, analogous to that of carbonates.

The lift force on a charged particle that translates and rotates in an electrolyte

Authors

Prof. Aditya Khair - Carnegie Mellon University

Ms. Bhavya Balu - Carnegie Mellon University

Abstract

The distortion of the charge cloud around a uniformly charged, dielectric, rigid sphere that translates and rotates in an unbounded binary, symmetric electrolyte at zero Reynolds number is examined. The zeta potential ζ of the particle is asserted to be small relative to the thermal voltage scale. It is assumed that the equilibrium structure of the cloud is only slightly distorted, which requires that the Peclet numbers characterizing distortion due to particle translation, $Pe_t = Ua/D$, and rotation, $Pe_r = \Omega a^2/D$, are small compared to unity. Here, a is the radius of the particle; D is the ionic diffusion coefficient; $U = |\mathbf{U}|$ and $\Omega =$

$|\boldsymbol{\Omega}|$, where \boldsymbol{U} and $\boldsymbol{\Omega}$ are the rectilinear and angular velocities of the particle, respectively. Perturbation expansions for small Pe_t and Pe_r are employed to calculate the non-equilibrium structure of the cloud, whence the force and torque on the particle are determined. In particular, we predict that the sphere experiences a force orthogonal to its directions of translation and rotation. This 'lift' force arises from the nonlinear distortion of the cloud under the combined actions of particle translation and rotation. The lift force is given by $\boldsymbol{F}_{\text{lift}} = \mathcal{L}(\kappa a)(\epsilon a^3 \zeta^2/D^2) \boldsymbol{U} \times \boldsymbol{\Omega} [1 + \mathcal{O}(Pe_t; Pe_r)]$. Here, ϵ is the permittivity of the electrolyte; κ^{-1} is the Debye length; and $\mathcal{L}(\kappa a)$ is a negative function that decreases in magnitude with increasing a . The lift force implies that an unconstrained particle would follow a curved path; an electrokinetic analog of the inertial Magnus effect.

Ion Association vs Ion Solvation and the Electrical Double Layer in Water-in-Salt Electrolytes

Authors

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Mr. Zachary A. H. Goodwin - Imperial College London

Mr. Sheng Bi - Imperial College London

Prof. Alexei Kornyshev - Imperial College London

Prof. Martin Bazant - MIT

Abstract

One goal for the next generation of lithium ion batteries is to replace the flammable and thermally unstable organic electrolytes used commercially with safer, more environmentally friendly options. Water-in-salt Electrolytes (WiSEs) are a promising class of electrolytes that have been recently developed as a viable option to attain this goal. WiSEs display expanded electrochemical stability

windows, while maintaining high ionic conductivity. These desirable properties arise in WiSEs due to their ultra-concentrated nature, leading to complex bulk properties and interfacial structure.

In this work, we study the crucial competition between ion solvation and ion association in WiSEs. This competition results in the emergence of *two ionic states*: participating and spectating, as well as *two water states*: free and hydrating. This partitioning becomes extremely valuable in understanding the ionic conductivity of WiSEs—dominated by participating ions—as well as understanding the electrochemical stability window of WiSEs—controlled by free water and interfacial structure. We observe this partitioning in molecular dynamics (MD) simulations for a variety of WiSEs across a range of high concentrations, and we formulate a continuum scale thermodynamic theory that describes the bulk partitioning of species into their various chemical states. Finally, we incorporate our bulk thermodynamic description of WiSEs into a modified Poisson-Boltzmann theory that is able to describe the complex EDL structure observed in our MD simulations. Our simulations and theory provide some the necessary insight for designing future WiSEs with better transport properties and stability.

Charge trapping at hydrophobic polymer-electrolyte interfaces enables efficient drop-based energy harvesting

Authors

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Mr. Niels Mendel - University of Twente

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Dr. Dirk van den Ende - Univ. Twente

Prof. Guofu Zhou - South China Normal University

Prof. Frieder Mugele - University of Twente

Abstract

Hydrophobic polymer surfaces spontaneously accumulate negative charge upon contact with water. Likewise, rolling drops on hydrophobic surfaces tend to leave traces of negative charge due to a poorly understood triboelectric charge transfer process. This phenomenon has recently been used to harvest energy from rolling drops. Here, we present an alternative droplet-based energy harvesting process, which relies on a dedicated charging process that deposits a substantially higher amounts of stable, permanently trapped charge on the polymer surface. We quantify the trapped charge density and its life time using electrowetting. The enhanced charge density enables more efficient conversion of droplet kinetic energy into electric energy based on transient variations of electrical capacitances due to varying drop shapes and positions upon impact on the surface. Synchronized high speed video imaging and electrical current measurements are used to confirm the proposed energy conversion mechanism.

Theory of electrokinetics and acid-base chemistry in porous electrodes for water desalination

Authors

Dr. Jouke Dykstra - Wageningen University

Abstract

Elektrokinetics and acid-base chemistry in membranes and porous electrodes

For many applications in the field of electrochemical engineering, transport of ions across ion-exchange membranes is important to evaluate. Often, the electrolyte contains various ionic species, and these ionic species undergo acid-base reactions. In this work we will show how we can model transport of ionic species and uncharged molecules through ion exchange membranes, considering that ions are subject to diffusional and migrational forces. Furthermore, we show how we can consider ongoing acid-base equilibrium reactions in our theoretical framework. These acid-base equilibria can be directly incorporated in the ionic mass balances. As a result, the model does not make

use of reaction rate constants, but only uses the pK value of the respective equilibrium [1].

Porous electrodes for water desalination

We will show how we can use this framework to model ion transport in Capacitive Deionization (CDI), an electrochemical separation process for water desalination. Capacitive Deionization (CDI) typically uses one porous carbon electrode that is cation-adsorbing and one that is anion-adsorbing. We will present an innovative CDI cell design with two anion-selective electrodes, in combination with a cation-selective membrane, and we show that this design continuously desalinates water [2]. A theoretical model, which includes ion transport across the single ion-exchange membrane, and ion adsorption in the pair of porous electrodes, is used to describe the data. To describe ion adsorption, the amphoteric Donnan model is used, which describes ion adsorption in electrical double layers located inside carbon micropores combined with the effect of chemical surface charge. We find that the theory describes experimental data well, both for the unmodified and the chemically modified anion-selective electrodes.

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Self-Charging Dielectric Elastomers

Authors

Prof. Thiago Burgo - Federal Univestity of Santa Maria

Prof. Fernando Galembeck - Unicamp

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Ms. Kelly Moreira - Federal Univestity of Santa Maria

Abstract

This work reports the rubber electrostatic potential due to repeated strain as a function of time for periods as long as the lifetime of the sample. Rubber potential depends on two main contributions: hygroelectricity added to the mechanochemical reactions evidenced by spectroscopy and microscopy/microanalytical experiments. Hygroelectricity produces fast periodic charging in phase with rubber strain, while a slower charging process is assigned to the mechanochemical reaction products, in conjunction with residual hygroelectricity. This result explains the significant negative potential displayed by rubber over long periods in the absence of any external applied voltage. These findings may contribute to improving dielectric elastomer performance in many applications that are currently of great interest in robotics and energy harvesting. Additionally, electric potential real-time measurements show desirable features as a tool for real-time, non-contact detection of rubber structural change and fatigue.

Free and Bound States of Ions in Ionic Liquids, Conductivity, and Underscreening Paradox

Authors

Prof. Guang Feng - Huazhong university of science and technology

Mr. Ming Chen - Huazhong university of science and technology

Mr. Sheng Bi - Imperial College London

Mr. Zachary Goodwin - Imperial College London

Prof. Eugene Postnikov - Kursk State University

Prof. Nikolai Brilliantov - University of Leicester

Prof. Michael Urbakh - Tel Aviv University

Prof. Alexei Kornyshev - Imperial College London

Abstract

Room temperature ionic liquids (RTILs) are cold ultra-dense ionic plasmas, in which the distances between cations and anions are of the order of their size. The rediscovery of them was a revolution in chemistry. With hundreds of RTILs synthesized, easily mixable, their 'cocktails' offer almost unlimited number of 'universal' or 'designer' solvents. However, despite many existing applications of RTILs as solvents and/or electrolytes, from catalysis to energy to nanotribology, rational utilization of their properties requires physical understanding of state and kinetics of ions in RTILs. A very important question is whether ions in RTILs 'freely' diffuse, or are rather 'bound' inside a cluster of ions.

In the reported work¹, using molecular dynamics (MD) simulations and theoretical analysis of ion dynamics, we not only confirm the existence of the widely speculated concept of 'free' and 'bound' states, but also unravel the laws of inter-conversion between them. A dynamic criterion has been proposed, based on the ion trajectory density, verified by two other methods, to determine the average portion of 'free' ions. It reveals that ~15-25% of ions of a typical RTIL-[BMIM][TFSI] are 'free', with their amount increasing with temperature following the Arrhenius law, in the range of 300-600K (for comparison, similar results are also obtained for other RTILs).

Our simulation results are in excellent agreement with experimental data on conductivity and diffusion coefficients. The predicted conductivity of RTILs, based on MD-obtained concentrations and diffusion coefficients of 'free' ions, well obeys Nernst-Einstein equation. These findings are rationalized based on developed kinetic theory, as well as they match an earlier proposed² 'collective-language'-based *narrow band ionic semiconductor concept*.

The identified substantial portion of 'free' ions contribute to the ionic conductivity and the formation of electrical double layers at electrified interfaces that lie in the basis of many applications of RTILs. The bespoke 'underscreening', thus, cannot be explained simplistically, in terms of 'minute amounts of free ions'.

Evaluation of the accuracy of Donnan-Manning theory for predicting ion exchange membrane permselectivity at elevated salt concentrations

Authors

Mr. Ryan Kingsbury - University of North Carolina at Chapel Hill

Prof. Orlando Coronell - University of North Carolina at Chapel Hill

Abstract

Ion exchange membrane (IEM) based processes are increasingly important for water purification and renewable energy generation and storage. In IEM-based processes, current efficiency is directly related to IEM permselectivity, which quantifies the extent to which the membrane permits the passage of counter-ions while excluding co-ions. Permselectivity depends on the process conditions (e.g., salt concentrations), but there is not currently an accurate, quantitative way of predicting IEM permselectivity, partly because of the inability to accurately predict ion activity and diffusion coefficients within the membrane. Recently, however, Manning's counter-ion condensation theory has been shown to predict ion activity and diffusion coefficients in IEMs with good accuracy under a broad range of salt concentrations. Accordingly, in this study, we evaluated whether Manning theory can be used in combination with Donnan exclusion theory to quantitatively estimate IEM permselectivity as a function of electrolyte concentration. We first measured the permselectivity of four IEMs over a range of salt concentrations and concentration gradients. We also measured the concentration of mobile salt sorbed by each membrane under the tested concentration gradients. Using these data and other experimentally measured membrane properties, we constructed a model based on Donnan-Manning theory to predict IEM permselectivity. We compare predicted and experimental permselectivity values, and identify experimental conditions and membrane parameters potentially associated with deviations of prediction from experiment. We also compare the accuracy of Donnan-Manning predictions with those obtained using the ideal Donnan exclusion model.

Metamaterials, Plasmonics and Electrochemistry: Tuning photonic functionalities in real time

Authors

Prof. Alexei Kornyshev - Imperial College London

Abstract

This talk will overview a new direction of research that can be conventionally called “electrochemical plasmonics”. It is based on voltage-controlled self-assembly of and electro-kinetic manipulations with arrays of plasmonic nanoparticles at electro-chemical liquid-liquid or solid-liquid interfaces, the optical properties of which can dramatically vary with assembly structure and density. The effects to be discussed were navigated by theory and have been experimentally realized by a team at Department of Chemistry of Imperial College; these refer to electro-switchable window-mirrors, tuneable colour mirrors, optical cavities, and ultrasensitive detectors of hazardous molecules or pollutants using novel self-assembling SERS platforms. One of the spectacular features of that area is demonstration that combination of correct physical chemistry of functionalized, charged nanoparticles in solutions and at electrodes, electrochemistry, and electrodynamics of nanostructured interfaces – work altogether exactly as expected, giving, however novel fascinating results. This opens a road towards a new class of electrotuneable optical metamaterials.

Targeting colloidal particle delivery into dead-end pores using solute gradients generated in situ

Authors

Dr. Huanshu Tan - University of California, Santa Barbara

Mr. Anirudha Banerjee - University of cal

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Dr. Afnan Mashat - Saudi A

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Prof. Todd Squires - University of California, Santa Barbara

Abstract

Particle and droplet transport into targets lies at the heart of many applications in a variety of fields including drug delivery, particle sorting, gas/oil recovery, and health industry. However, in micro-scale systems, the transport of particles into or out of dead-end pores is hindered by the inability to flow fluids into them.

Diffusiophoresis – particle migration driven by solute gradients – provides an efficient way to solve this problem, as colloidal particles can migrate along a solute gradient into or out of confined geometries. Here, we explore strategies to generate solute fluxes *in situ*, e.g. to drive particles towards ‘target’ sites within a pore. We anticipate practical applications, both directed delivery of colloidal particles and in autonomous target detection.

Numerical analysis of three-dimensional electrohydrodynamic instability in crossflow

Authors

Mr. Yifei Guan - University of Washington

Prof. Igor Novosselov - University of Washington

Abstract

The study focuses on the electro-hydrodynamic (EHD) instability between two parallel plates in the presence of cross-flow. Second-order accurate Lattice Boltzmann Method with two-relaxation time model is used in the 3D numerical simulation¹. In the absence of cross-flow, the base-state solution is hydrostatic, and the electric field is one-dimensional. The solution becomes unstable equilibrium when a sufficiently strong charge injection is introduced. Perturbed

by 2D (rolling) or 3D (square) patterns, the electroconvection vortices (ECV) develop based on the most unstable modes. The growth rate and the unstable modes are obtained by performing dynamic mode decomposition (DMD) on the transient numerical solutions. The growth rate is similar to the rate obtained by a linear stability analysis. Once the steady-state solution with ECV is obtained, a Couette or Poiseuille cross-flow is introduced. The cross-flow applied to 3D flow patterns suppress vortices in the direction of the cross flow, leading to pattern transition from square to oblique 3D, to 2D rolling patterns in the stream-wise direction.

A non-dimensional parameter is derived to characterize the transition from the 3D to 2D flow pattern.

$$Y = \rho_0 \varphi_0 H / \mu u_{ext}$$

where ρ_0 is the charge density, φ_0 is the electric potential, μ is the dynamic viscosity of the fluid, H is the distance between two plates and u_{ext} is the external flow velocity in crossflow direction. Similar to previous presented 2D analysis², critical values of Y are obtained to characterize hysteresis behavior of the 3D fluid system with ECV.

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Automated In-Situ Wettability Characterization on Reservoir-on-a-chip Using Deep Learning

Authors

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Dr. Sehoon Chang - Aramco Services Company, Aramco Research Center – Boston

Prof. Anthony R. Kavscek - Stanford University

Abstract

Wettability of porous media and its influence on the efficiency of wetting- or non-wetting phase displacement is a key factor in estimating recovery efficiencies of hydrocarbons. As a result, understanding wettability alteration mechanisms in an oil-brine-rock (OBR) system, including multicomponent ion exchange and electrical double layer interaction between rock and oil, has attracted increasing interest. Reservoir-on-a-Chip (ROC) methods using microfluidic devices is a useful laboratory platform for the direct visualization of pore-scale fluid transport in complex geometries. Studies using microfluidic devices, so called micromodels, in turn potentially brings better understanding of wettability alteration mechanisms and their effects on pore-level hydrocarbon displacement efficiency. Recently, we assessed performance of various chemical enhanced oil recovery surfactants using calcium carbonate (CaCO_3) coated micromodels. High resolution imaging techniques along with labeling fluorescence dyes of water and oil phases enabled visualization of wettability alteration while surfactants interacted with the water-crude- CaCO_3 coated surface.

Pore-level wettability alteration and its impact on estimating phase desaturation at larger scale is complex because the sensitivity to pore-scale details and the large number of coupled mechanisms, and their governing parameters vary over a wide range of scales. Consequently, it is necessary to visualize pore-scale phenomena, at the same time; achieve a systematic way to study the larger domain of porous media that consists of complex interplays between surface

and reservoir fluids at the smaller sub-domains. Advanced imaging techniques allow rapid acquisitions of large number of high-resolution pore-level images during experiments. However, it is generally not feasible to perform quick but thorough investigations of large sample image datasets over a large field of view (FOV). This limits a full characterization of the complex interplay between preferential flow path, wettability alteration, and oil displacement occurring the entire domain of micromodel. Therefore, the present work elucidates both the experimental procedure to prepare data (pore scale images of oil- and water-wet) and the training of novel deep-learning algorithm for the binary classification of wettability. Experimentally, image datasets were prepared from the visualization of the saturation profile of two phases (mineral oil and water) using in-house fabricated micromodels with Sandstone- and Carbonate-like pore structures. The datasets consist of 6400 color images in 4 classes for sandstone (water- or oil-wet) and carbonate rock pattern (water or oil-wet), with 1600 images per class. 3000, 100, and 100 images per each rock pattern were used as training, validation, and test set, respectively. We trained and optimized Convolutional Neural Network (ConvNet), on the training and validation data set. The best ConvNet model shows the test set accuracy of $99\pm 1\%$ for binary surface wettability classification for both rock patterns. We believe that our trained ConvNet has a great potential to serve as a time-efficient method for real-time monitoring of wettability alteration during micromodel EOR experiment, for instance ionically tuned water or surfactant injection.

Electrokinetic control of miscible flow instabilities in porous media

Authors

Dr. Amin Amooie - MIT

Dr. Mohammad Mirzadeh - Massachusetts Institute of Technology

Prof. Martin Bazant - MIT

Abstract

We present a modeling study of the control of miscible interfacial instabilities in porous media under the coupled action of pressure and concentration gradients and electric field. When two fluids of different physical properties such as density, viscosity, or electrolyte concentration contact each other, interfacial instabilities may occur whereby the lighter or more conductive fluid forms finger-like patterns into the other fluid. Here, we first study the dynamics of miscible viscous fingering, and show how electric current applied in the right amount and direction can induce or suppress instabilities depending upon its cooperation with advective and diffusive fluxes.

Second, we strive to harness these electrokinetic feedbacks for improving CO₂ storage—via dissolution-driven convection—in salt-containing, water-filled porous formations (i.e. saline aquifers) subject to electric fields. We model the coupled hydro-electro-chemical processes that occur upon the reactivity of dissolved CO₂ with both pore water and rock surface. We find electrokinetic flows may either lead to a combined free and forced convection (mixed convection) or strictly strengthen the density-driven convection, thereby enhancing the dissolution and mixing processes.

Our results provide a new perspective into how electrokinetic phenomena may control the dynamics of miscible hydrodynamic instabilities in porous media with applications to different energy and environmental problems.

Manipulating the Belousov-Zhabotinsky reaction with silver-silver bromide electrodes

Authors

Mr. Arnaldo Rodriguez-Gonzalez - Cornell University

Prof. Brian Kirby - Cornell University

Abstract

The Belousov–Zhabotinsky (or B-Z) reaction is arguably the most prolific example of an autocatalytic chemical reaction, in which different chemical components oscillate in concentration over time. To manipulate these

oscillations, many scientists utilize organic compounds to indirectly regulate the production of bromide ions, a key reagent in the B-Z reaction. We describe our efforts to directly manipulate the concentration of bromide ions in the B-Z reaction using silver-silver bromide electrodes, which can potentially lead to localized fine-tuning of the oscillatory behavior of this reaction, and describe plausible electrochemical models for this process.

Low dispersion flow cell with asymmetric redox active electrodes for selective removal of ionic pollutants

Authors

Dr. ALI HEMMATIFAR - Massachusetts Institute of Technology

Mr. Kai-Jher Tan - Massachusetts Institute of Technology

Prof. T. Alan Hatton - Massachusetts Institute of Technology

Abstract

The lack of clean water is a worldwide concern and one of the global challenges of the century. The twofold issue of water scarcity and poor quality aggravate the situation even further. Naturally occurring toxins and contaminants currently pose severe health threat in regions such as southeast Asia, south America, and others. In addition, traces of man-made micropollutants and contaminants resulted from municipal, industrial, and agricultural activities can be found in various water sources: from groundwater, lakes, and rivers to even sources used for human consumption. Such contaminants might include highly toxic organic ions such as chemical wastes, pesticides, and pharmaceuticals.

Electrosorptive separation of the contaminants, compared to membrane-based and thermal processes, provides unique opportunities in water purification and environmental remediation efforts: higher scalability, reusability, and enhanced ion selectivity. Specifically, surface-functionalized capacitive desalination as well as redox-mediated electrodes have demonstrated selective ion removal. Among these, asymmetric redox systems are of great interest due to their high adsorption capacity and tunable selectivity.

Although fundamental research on redox-active materials has shown feasibility of selective electrosorption in batch mode, a system-level study with continuous flow operation and with practical scale is still lacking. To address this, we here demonstrate our effort in design and fabrication of a novel, low-dispersion flow system which consists of multiple flow cell modules with asymmetric redox-active electrodes. Each module has a pair of electrodes coated with anion- and cation-selective redox moieties, a pair of titanium current collectors, and an inlet and outlet ports. In an effort to minimize the flow mixing and dispersion effects during operation (a prevailing limitation of the current flow systems) and to minimize the module footprint, we fabricated the modules in spiral electrode configuration. Electrodes are spirally-wound around an electrically-insulating core and are separated with porous mesh spacers, allowing the solution to flow between the electrode. Such design, which resembles the packed bead reactor, enables highly effective electrosorption due to uniform flow and residence time inside the module.

Further, we present results of in-situ and ex-situ electrochemical analyses such as cyclic voltammetry and impedance spectroscopy and optimize the current and operating voltage window of our asymmetric redox flow cell for maximum robustness. We present results of ion-selective adsorption measured with UV-Vis and conductivity sensors and the corresponding current and voltage profiles.

In short, we demonstrate a low-dispersion, scalable, and robust solution to the challenge of selective contaminant removal. Additionally, our spirally-wound cell with asymmetric redox electrodes shows a great flow-efficiency with minimal flow mixing or dispersion inside the module, extremely favorable in wide range of water purification applications.

Capacitive deionization of water: Resonance and selective extraction

Authors

Dr. Ashwin Ramachandran - Stanford University

Mr. Diego Oyarzun - Stanford University

Prof. James Palko - University of California Merced

Dr. Steven Hawks - Lawrence Livermore National Labs

Dr. Patrick Campbell - Lawrence Livermore National Labs

Dr. Michael Stadermann - Lawrence Livermore National Labs

Prof. Juan Santiago - Stanford University

Abstract

Presented will be analytical models and experimental studies of capacitive deionization (CDI) for desalination and toxin removal. Well-designed CDI cells are a promising alternative to existing desalination technologies, including reverse osmosis. This is particularly true for the desalting of water with low to moderate levels of salinity (brackish water), where CDI is most efficient. CDI cell capacity scales approximately linearly with material requirements and capital costs, and these systems require negligible supporting infrastructure. A CDI cell uses one or more pairs of oppositely charged porous electrodes (typically carbon) within a housing fitted with a single inlet for feed water and a single outlet. A maximum of about 1.2 V potentials are applied between electrodes, driving ionic species in solution toward electrode surfaces, where they are capacitively and reversibly retained.

In the area of desalination, we developed a theory around and experimentally demonstrate new operation modes for CDI including sinusoidal electrical forcing. We use a dynamic system analysis approach and quantify the frequency response of CDI effluent concentration. We explore the coupling between electric charge, ionic charge, and mass transport and demonstrate that sinusoidal voltage forcing functions can achieve resonance-type operation for CDI. Operation at resonance results in an optimal balance between absolute amount of salt removed (in moles) and avoidance of dilution of the feed and brine streams.

In the area of toxin removal, we developed specialized CDI cells for selective toxin removal from water. We functionalize active carbon electrodes with ion-selective functional groups. We developed an experimentally validated model

that combines a Donnan treatment for electric double layers (EDL) and electrosorption Langmuir-type equilibria. We built and demonstrated a CDI cell for nitrate removal and used ion chromatography to quantify performance. Functionalization of activated carbon electrodes provides a selective ion capture system with that can be regenerated with applied voltage. We demonstrated a nitrate-specific functionalization with up to 6.5-fold cycle selectivity.

Shock Electrodialysis for Ion-Selective Water Purification

Authors

Dr. Kameron Conforti - MIT

Mr. Mohammad Alkhadra - MIT

Dr. Tao Gao - MIT

Ms. Huanhuan Tian - MIT

Prof. Martin Bazant - MIT

Abstract

Shock electrodialysis is an emerging method of water desalination, based on separating fluid streams on either side of a deionization shock wave propagating through a charged porous medium under over-limiting current. This talk will introduce the basic physics of shock ED and demonstrate promising new applications in water treatment. For dilute feed streams, shock ED is capable of complete (>99.99%) salt removal with high (>85%) water recovery, which we apply to the removal of cobalt and cesium ions from nuclear waste. High (>90x) selectivity for multivalent ions is also illustrated by the removal of magnesium and lead from sodium chloride solutions. High selectivity at low salt concentrations leads to ultra low energy costs (pennies per meter cubed), which could lead to the first practical solution for lead removal from contaminated pipes, as in Flint, Michigan. This work also raises fundamental questions about extreme nonlinear electrokinetics in porous media, at up to 25 times the diffusion-limited current

Electrostatic and density correlations in the electrical double layer

Authors

Mr. Pedro de Souza - MIT

Prof. Martin Bazant - MIT

Abstract

The classical mean-field Poisson-Boltzmann theory breaks down for (i) concentrated electrolytes due to crowding effects and non-ideal thermodynamics, and (ii) low dielectric constant solvents, multivalent ions, and highly charged surfaces due to electrostatic correlations. Typically, theories either include these effects with modifications that neglect the density and electrostatic correlations, for example, with local density approximations, or they include these effects with complicated density functional methods based on perturbative expansions or weighted density approximations. Here, we demonstrate how to incorporate correlation effects in a simple free energy functional formulation, in which the free energy density appears in terms of local values of the ion or solvent density and their derivatives. The structure of the interface emerges from this simple formulation, which can be solved with a system of coupled ordinary differential equations, or solved analytically in the linear regime. For electrostatic correlations, the gradient expansion of the electrostatic potential leads to overscreening of surface charge. We demonstrate the effects of correlations in the fluid structure at an interface, in the interactions of charged colloidal particles, and in electrokinetic phenomena.

Thermodynamics of signal conduction in neurons

Authors

Mr. Aymar de Lichtervelde - Wa

Mr. Pedro de Souza - MIT

Prof. Martin Bazant - MIT

Abstract

Nervous transmission is associated with electrical, mechanical and thermal responses. In particular, production and subsequent absorption of heat is observed during the conduction of the action potential along neurons. The reversible release of capacitive energy stored across the cell membrane appears as a simple and consistent explanation, as proposed in the “condenser theory.” However, this hypothesis has not been analyzed beyond the analogy between the cell membrane and a parallel plate capacitor (i.e. a condenser). In this work, we revisit the condenser theory using a detailed electrostatic model of the cell membrane and electrical double layers that form on each side of it. Based on this biophysical model and dielectric theory, we derive expressions for free energy and entropy changes associated with the depolarization of the membrane by the action potential, which give a direct measure of the heat produced and absorbed by neurons. We show how the density of surface charges on both sides of the lipid bilayer impacts such energy changes. We re-interpret entropy changes in the membrane in the light of new experimental data. Finally, considering a typical action potential, we show that if the membrane holds a bias of surface charges that makes the internal side of the membrane 0.05 C m^{-2} more negative than the external side, the size of the heat predicted by the model reaches the range of experimental values. Based on our study, we identify the change in electric energy of the membrane as the primary mechanism of heat production and absorption by neurons during nervous conduction

Next-Generation Desalination Membranes

Authors

Prof. Menachem Elimelech - Yale University

Abstract

Water scarcity is one of the greatest global crises of our time. Increasing water supply beyond what is available from the hydrological cycle can be achieved by seawater desalination and wastewater reuse. Highly effective, low-cost, robust

technologies for desalination and wastewater reuse are needed, with minimal impact on the environment. However, progress in current state-of-the-art water purification membranes has been limited due to inherent limitations of conventional membrane materials. We will first discuss the state-of-the-art of existing membrane technologies for water purification and desalination, highlight their inherent limitations, and establish the critical needs for next-generation membranes. We will then critically analyze recent approaches involving nanomaterials to advance membrane desalination technologies. Lastly, we will describe molecular-level design approaches to fabricate highly selective membranes, focusing on novel materials such as aquaporin, synthetic nanochannels, and self-assembled block copolymers.

Electrochemical transformation of crude oils in electrokinetic recovery

Authors

Prof. Ehsan Ghazanfari - University of Vermont

Prof. Sibel Pamukcu - Lehigh University

Prof. Mesut Pervizpour - Lehigh University

Abstract

Electrically assisted transport of hydrocarbon compounds in natural porous media has generally been investigated for environmental mitigation of contaminating oils. The same fundamental principles apply to electrokinetic oil recovery. There are key contributing factors to the oil production under applied DC current among which reduction in interfacial tension between the oil and water as well as reduction of oil viscosity due to transformation of the oil through electrochemical reactions.

In this paper, reduction of interfacial tension between formation water and oil, and reduction in oil viscosity are discussed and investigated through floor scale laboratory experiments on synthetic formation matrices. In these experiments, constant direct current was applied for 107 days. Voltage, current, and oxidation reduction potential (ORP) were measured directly at eight different sections

along the center line of each test cell through designated ports. Formation samples were taken periodically for gravimetric (oil-water content), UV and FTIR analysis following any marked changes observed in the ORP. At the end of 107 days of treatment, the cells were dismantled and sufficient formation oil was extracted from the sampling locations to run FTIR, SARA, and viscosity analysis.

The results of these experiments showed that, there is a direct correlation between the oxidation reduction potential (ORP) of the formation and the asphaltene content of the formation oil. For neutral pH conditions, a reductive environment promoted reduction in asphaltenes which in turn affected the interfacial surface tension between formation water and oil as well as the viscosity of the crude oil. The results showed about 70% and 25% drops in the viscosity of heavy crude oils at the anode and the cathode regions of the test matrices, respectively compared to their initial values.

Faradaic Modulation of Redox Polymer-Functionalized Electrodes for Controlled Electrosorption

Authors

Mr. Sahag Voskian - MIT

Ms. Fan He - Massachusetts Institute of Technology

Prof. T. Alan Hatton - MIT

Abstract

The growing crisis enveloping the world as a result of water shortages and global climate change demands strong action to mitigate environmental contamination and greenhouse gas emissions. Energy efficient technologies are called for to address these burning issues, including new separation approaches that rely on green energy, such as electricity from renewable solar or wind resources. We have been exploring the use of Faradaically controlled sorption media for the selective recovery or removal of target compounds from both aqueous and gaseous feeds, and demonstrated that they could have significant advantages over other approaches to separations. Specifically, we rely on species-specific interactions between targeted compounds and electrochemically modulated

redox polymers on functionalized electrodes to attain high selectivity in electrosorptive separation processes. Under certain applied potentials, the fraction of immobilized moieties activated by Faradaic oxidation or reduction reactions depends on the degree to which they are stabilized by interactions with the targeted species, such that targeted compounds that have stronger interactions with the redox groups lead to a greater degree of activation, and hence higher electrosorptive capacity. Two systems are of interest, one a liquid phase for capture of, e.g., organic anions, and the other a gas phase from which CO₂ is removed by electrosorption.

This talk will focus on the dynamics of these electrosorption processes under flow conditions, and the interplay between Faradaic reactions, localized currents, and the development of adsorption fronts.

Holistic molecular imaging and rapid phenotyping of complex biological systems

Authors

Prof. Kwanghun Chung - MIT

Abstract

Holistic measurement of diverse functional, anatomical, and molecular traits that span multiple levels, from molecules to cells to an entire system, remains a major challenge in biology. In this talk, I will introduce a series of technologies including CLARITY (Nature, 2013), SWITCH (Cell, 2015), MAP (Nature Biotechnology, 2016), stochastic electrotransport (PNAS, 2015), and SHIELD (Nature Biotechnology, 2019) that enable integrated multiscale imaging and molecular phenotyping of both animal tissues and human clinical samples. I will discuss how we engineer (1) the physicochemical properties of brain tissues, (2) molecular interactions, and (3) molecular transport all together to achieve integrated brain-wide molecular phenotyping at unprecedented speed and resolution. I will also discuss how these tools can be deployed synergistically to study a broad range of biological questions. We hope that these new technologies will accelerate the pace of discovery in biomedical research.

Microslit Electrokinetic Analyses to Explore Soft Macroscopic Interfaces

Authors

Prof. Ralf Zimmermann - Leibniz Institute of Polymer Research Dresden

Prof. Carsten Werner - Leibniz Institute of Polymer Research Dresden & Technische Universität Dresden

Abstract

Interfacial charge characteristics of soft engineered matter exposed to aqueous environments are critically important in several emerging technologies, however, remain difficult to determine. Microslit electrokinetic analysis has been established as an extended streaming potential/streaming current methodology that provides the quantification of surface conductance and, by that, analytical access to ionization processes, ion-binding, and polymer segment distribution of hydrodynamically stagnant interfacial layers (1). Advantageously, the microslit experiment and sample format facilitate complementary analyses, such as physical layer thickness measurements and surface spectroscopies (2-5).

Our contribution will elaborate on options of microslit electrokinetic experiments -in combination with theories of soft diffuse interfaces relying on the provided data (6-8)- for unraveling interfacial charging and structural features of various (bio)polymeric materials. Examples to be discussed include synthetic -such as stimuli-responsive- polymer materials, biopolymeric and biohybrid hydrogels, polymer brushes, polyelectrolyte multilayers, and supported bilayer lipid membranes (9-13).

We will conclude by highlighting experimental challenges of microslit electrokinetic analyses as well as the necessity of theoretical work to further exploit the charging and charge compensation phenomena of hydrodynamically distinct interfacial regions at soft macroscopic interfaces.

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Spatio-temporal morphogen gradients to direct cell-fate decisions in glycosaminoglycan-based hydrogels

Authors

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Dr. Felix Schrön - Leibniz Institute of Polymer Research Dresden

Dr. Yanuar D. P. Limasale - Leibniz Institute of Polymer Research Dresden

Dr. Christoph Hentschel - Leibniz Institute of Polymer Research Dresden

Dr. Passant Atallah - Leibniz Institute of Polymer Research Dresden

Dr. Uwe Freudenberg - Leibniz Institute of Polymer Research Dresden

Prof. Carsten Werner - Technische Universität Dresden

Abstract

Glycosaminoglycans (GAGs) are a class of linear polysaccharides that are ubiquitous in the extracellular matrix (ECM) and on cell surfaces. Due to their ability to effectively bind, protect, and sustain the release of morphogens, GAGs are increasingly used in the design of ECM-mimicking hydrogels to stimulate tissue formation and regenerative processes via specifically orchestrated cell-instructive signals (1). The specificity and strength of morphogen-GAG interactions are largely governed by the number and spatial distribution of negatively charged sulfate groups carried by GAGs (2,3). Presenting data from biomolecular interaction analysis (4), numerical simulations of molecular transport and binding, and 3D cell culture experiments, we demonstrate how the spatio-temporal presentation of morphogens to cells in hydrogels formed from poly(ethylene glycol) and heparin (starPEG-heparin hydrogels) can be modulated by varying the heparin concentration and sulfation pattern. In particular, we show how the migration and morphogenesis of human mesenchymal stem cells can be controlled by growth factor gradients in 3D printed zonal hydrogels. We further provide insights into the morphogenesis of human umbilical vein endothelial cells into capillary networks and how this process is influenced by the concentration and sulfation of the heparin.

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Interpretation of the effect of particle size on fast aggregation rate using structural layer model

Authors

Dr. Hongyan Sun - Chinese Academy of Sciences

Prof. Daosheng Deng - Fudan University

Abstract

A laser diffraction instrument was used to detect the change of scattered light intensity at the scattering angle of 0.0144° to get the value of aggregation rate. An interesting finding is that when the particle size is less than 190 nm, the fast aggregation rate of silica particles reduces by the orders of magnitude compared with the theoretical value. A hypothesis is proposed that there existing a structural layer on silica surfaces, where the short-range repulsive force hinders the collision between particles, resulting in reduction of the fast aggregation rate. Based on the hypothesis, it successfully explained anomalous phenomena, which don't conform to DLVO theory, such as the reduction of fast aggregation rate of small particles under high ionic strength and the variation of the rate as a function of pH. Therefore, the classic Smoluchowski formula was modified by introducing the structural layer repulsion and the thickness of structural layer under different conditions was obtained. The results showed that the smaller the particle was, the thicker the structural layer would be. What's more, the distance where the interaction force between two particles is the minimum is exactly twice the thickness of structural layer for particles whose size are below 190 nm. Besides theoretical calculation, coagulation experiments were operated to further verify the rationality and accuracy of the hypothesis.

Ion concentration polarization in micro/nanofluidic platforms

Authors

Prof. Sung Jae Kim - Seoul National University

Abstract

Recent advances in micro/nanofabrication technique enable one to study fundamental nanoscale electrokinetics and develop innovative engineering applications in micro/nanofluidic platform. While concentration polarization (CP) conventionally refers a polarized electrolyte concentration across a nanoporous membrane under dc bias in a macroscale platform such as electrodialysis system, ion concentration polarization (ICP), which is similar phenomena as CP has been dealt in micro- or nano-scale confined environment. Thus, surface driven phenomena such as surface conduction and electroosmotic flow become dominant in this environment due to high surface to volume ratio.

In this presentation, key differences between CP and ICP will be discussed by focusing the influence of surface conduction and electroosmotic flow on a perm-selective nanojunction between microchannels. Furthermore, unique engineering applications using the micro/nanofluidic platform will be introduced as well, for example, high efficient biomolecular selective preconcentrator and portable artificial kidney device.

Understanding the Impact of Hybrid Nano Acid Fluid (HNAF) Pulsed with Electrokinetic (EK) stimulation in Tight Carbonate Reservoirs

Authors

Dr. Mohamed Haroun - Khalifa University of Science and Technology

Prof. George Chilingar - University Southern California

Abstract

1. Objectives/Scope

This study characterizes the impact of hybrid nano-acid fluids (HNAF) to improve oil recovery from tight carbonate reservoirs. While acidizing creates continuous channels (wormholes), nanoparticles enhance this effect due to their capability in penetrating through the tight pore throat sand adsorbing on the surface of the formation. In addition, the application of HNAFs with pulsed electrokinetics

(EK) effectively stimulates the tight formation as confirmed by dual energy computed tomography (DECT) scan, creating efficient wormholes.

2. Methods, Procedures, Process

The following study is divided into two stages to investigate the performance of HNAF in tight formations. Compatibility and IFT tests were performed to help in identifying the concentration and combination of the novel HNAF stimulation fluids. A total of 12 Carbonate core-plugs were flooded with the HNAF formulations with and without EK and reproduced to confirm their respective performance. Spontaneous imbibition was conducted to demonstrate the effect of nanoparticles on wettability alteration. DECT, NMR, and Zeta potential tests were conducted before and after each core flooding (CF) experiment to rank the combined mechanisms observed from the novel HNAFs.

3. Results, Observations, Conclusions

HNAF formulations tested, included (HNAF1), (HNAF2) and (HNAF3), generated a significant IFT reduction under HPHT conditions from 18 dyne/cm (formation water and oil) to 3.14, 2.89, and 4.14 respectively.

When conducted with sequential application of EK, HNAF1 observed higher dominance as compared to HNAF2, which was followed by HNAF3, in terms of displacement efficiency (DE) and permeability enhancement (PE). However, during pulsed simultaneous application of EK, HNAF1 followed by HNAF3 and HNAF2 were confirmed to maximize both DE and PE.

The DE and PE averaged at 9% and 180% during sequential application. It was further observed that 13.5% and 176% during simultaneous application. The displacement efficiency recorded a significant increase in the case of simultaneous versus sequential while requiring 27% less pore volumes injected.

The zeta potential verified the observed CF ranking order through matched shifts in zeta potential before and after CF which confirms significant alteration in wettability post flooding. The DECT further verified permeability enhancement by virtue of wormhole imaging while NMR recorded a 32% increase of pore size distribution from micro pore throats to mesopore throats, thus confirming a significant increase in depth of penetration with the tested novel HNAFs.

4. Novel/Additive Information

The summary of the results of research shows promising potential to overcome the limitations reported from the previous studies and have matured the understanding of the application of HNAFs in tight carbonate reservoirs. This integrated study has assisted in the successful formulation of the EK assisted HNAF in lab scale.

Relationship Integrating Zeta Potential and Displacement Efficiency: A Novel Approach Towards Smart Waterflooding Mechanism

Authors

Dr. Mohamed Haroun - Khalifa University of Science and Technology

Prof. George Chilingar - University Southern California

Abstract

Objectives/Scope:

As an enhanced oil recovery (EOR) technique, smart water flooding has demonstrated positive results in multiple laboratory and field applications. This investigation presents a novel EOR technique on carbonate reservoirs using smart waterflooding combined with Electrokinetic enhanced oil recovery (EK-EOR).

Implementation of EK-EOR, combined with smart water flooding may enhance the oil/rock/brine interaction optimizing in such a way that the wettability can be altered from oil-wet state to a water-wetstate.

Methods, Procedures, Process:

This novel investigation focuses on wettability alteration in carbonate core plugs, by injecting different brines with and without EK. Low direct current was applied sequentially and simultaneously to investigate the incremental oil recovery. Zeta potential was measured for the formation water (FW) saturated and aged samples for a pH range of 6-8 which is representative to the reservoir

range. Post-core flooding, a zeta potential gradient was obtained for the inlet, middle and the outlet of the core sample. The zeta potential at the inlet were then correlated to displacement efficiency (DE) for the different brines employed. To understand the relation better between oil displacement and change in zeta potential, two new indexes have been introduced – Oil index (O_I) and Zeta Index (ζ_I). The Zeta index represents the change in surface charge pre and post flooding compared to original 100% FW saturated reservoir rock (inlet).

Results, Observations, Conclusions:

EK-assisted smart water flooding resulted in higher and accelerated displacement efficiency (75%) compared to low salinity flooding without EK (72.5%). A strong relation has been observed between displacement efficiency and shift of surface charge from oil wet to water wet. There was a clear increase in the zeta potential post flooding with the surface charge becoming more positive compared to the -12mV in inlet of aged sample indicating a shift towards water wet.

Analysis of the Zeta and Oil index indicated a very high positive correlation coefficient with an R^2 of 0.88. A total recovery of 72.47% was observed with a Zeta Index of 0.1 without the application of EK. Core flooding experiments with EK showed Zeta Index going well below 0 with an average recovery of 75%. This extra shift in zeta potential index may be attributed to the application of EK.

Novel/Additive Information:

Our study is unique as we introduce two new indexes which are Oil index (O_I) and Zeta Index (ζ_I) to understand the relationship between oil displacement and change in zeta potential. This can lead to better understanding of the underlying mechanisms within EOR techniques specifically in terms of EK-EOR.

Electrokinetic Induced Wettability Alteration in Carbonates

Authors

Mr. Amani Alghamdi - EXPEC Advanced Research Center

Abstract

In this experimental investigation, the impact of electrokinetic induced wettability alteration in carbonates was studied by measuring zeta potentials at calcite/brine and crude oil/brine interfaces using phase analysis light scattering technique. Three surfactants (two anionic and one amphoteric) and two types of alkalis (NaOH and Na₂CO₃) were used at a dilute concentration of 0.1 wt%. Three different low salinity water recipes representing Smart Water (10-times reduced salinity seawater), NaCl brine and Na₂SO₄ brines were chosen at a fixed salinity. Deionized water was also used to provide the baseline for comparison.

The results showed that alkali can increase the magnitude of zeta potentials at both interfaces towards more negative for Na₂SO₄ brine. However only slight increase in negative zeta potentials were observed with NaCl brine.

Na₂CO₃ effects on the zeta potential of calcite is found to be more pronounced when compared to NaOH due to the availability of carbonate ions as potential determining ions. In contrast, NaOH showed an improved effect on the zeta potentials of crude oil as NaOH is a stronger alkali to favorably result in the dissociation of the acids from crude oil. Both the anionic surfactants increased the magnitude of negative zeta potentials at the interfaces by almost same order of magnitude. The negative zeta potentials of calcite and crude oil were increased the most with anionic surfactant in NaCl brine. Smart Water showed relatively higher negative zeta potentials for calcite when compared to Na₂SO₄ brine in the presence of anionic surfactant. The amphoteric surfactant did not increase the magnitude of the negative zeta potential for both the interfaces. These results indicate that Na₂SO₄ brine is better suited with alkali whereas NaCl brine and Smart Water can synergistically combine with anionic surfactant to electrokinetically induce wettability alteration in carbonates.

This work for the first time evaluated electrokinetic induced wettability alteration effects caused by chemicals and changing water compositions in crude oil-brine-carbonate systems. The new knowledge gained from this electrokinetic study will provide useful guidelines on how to select right water chemistries and most effective chemicals for water flooding and chemical enhanced oil recovery processes in carbonate reservoirs.

Charge Screening and Electrokinetic Phenomena with Strongly Correlated Ions

Authors

Mr. Amir Levy - MIT

Mr. Pedro de Souza - MIT

Mr. Michael McEldrew - MIT

Prof. Martin Bazant - MIT

Abstract

The classical mean-field theory of electrokinetic phenomena assumes of perfect charge screening by a continuous cloud of excess counter-ions, leading to electroneutrality at the scale of the Debye screening length. This assumption makes no sense, however, in two common situations where the expected number of ions in the “cloud” is less than one! 1) For “3d correlated screening” in concentrated electrolytes, the Debye length becomes smaller than the nearest neighbor distance between ions (and in ionic liquids, smaller than the ion size), and over-screening charge oscillations arise. 2) For “1d correlated screening” in dilute electrolytes confined to charged nanopores, the nearest neighbor distance becomes larger than the pore size, and ions form an expanded chain that violates local electroneutrality. This talk will introduce simple mathematical models of both of these situations, which are able to predict puzzling electrokinetic phenomena, such as electrophoretic mobility reversals and anomalous conductance of nanotubes.

Electro-osmosis in Liquid Foam

Authors

Dr. Baptiste Blanc - Brandeis University

Dr. Oriane Bonhomme - Université Lyon 1-CNRS

Prof. Laurent Joly - Université Lyon 1-CNRS

Prof. Christophe Ybert - Université Lyon 1-CNRS

Prof. Anne-Laure Biance - Université Lyon 1-CNRS

Abstract

Investigating electrokinetic transport in a liquid foam is at the confluence of two well developed research areas. On one hand, the study of electrokinetic flows (i.e. surface-driven flows generated close to a charged interface) is fairly well understood in regards the solid/liquid interface. On the other hand, the flow of liquid in a 3D deformable network, i.e a foam, under a volume force such as gravity has been thoroughly studied over the past decade. The overlapping zone of these two frameworks is of great interest for both communities as it gives rise to challenging new questions such as: what is the importance of the nature of the charged interface, created by mobile and soluble surfactants in the case of foam, on electrokinetic transport? How does a foam behave when submitted to a surface-driven flow? Can we compensate a volume-driven flow, i.e. gravity, by a surface-driven flow, i.e. electroosmosis? In this work, we will explore these questions on two different scales: a surfactant laden interface and a macroscopic foam. I will first present an experimental study of the electroosmotic flow generated by one soapy interface. I will then discuss results obtained from a molecular dynamics simulations of nanobubbles covered with surfactants. Finally I will highlight how the design of electrodes is crucial to observe the electroosmosis in liquid foam and present some results on the behavior of such material under the application of an electric field.

Red-ox Responsive Hydrogel

Authors

Dr. Baptiste Blanc - Brandeis University

Prof. Zhenkhun Zhang - Nankai University

Prof. Bing Xu - Brandeis University

Prof. Hyunmin Yi - Tufts University

Prof. Seth Fraden - Brandeis University

Abstract

Yoshida developed a polyelectrolyte gel in the late nineties that experiences cyclic swelling and deswelling changes without external stimuli. This self oscillating gel contains a catalyst involved in the Belousov Zhabotinsky (BZ) reaction, an oxydation-reduction cyclic reaction, leading to a cyclic change of solubility of the gel. Our goal is to maximize the mechanical force generated by such an hydrogel during its transition from the reduced to the oxidized state. We envision this system as the building block for soft matter robots directly converting chemical energy into mechanical energy.

We focus our talk on a new synthesis method for producing red-ox responsive gel. This technique offers high modularity in the gel composition and in its functionalization with a red-ox responsive molecule. We present simple experimental techniques to measure its density, bulk modulus, timescale of swelling and catalyst concentration. This measurement enable us to calculate the force generated during the oxidation of such redox gel.

Ionic current magnetic fields in charged 3D nanoslits

Authors

Prof. Abraham Mansouri - Higher Colleges of Technology

Abstract

Internal and external magnetic fields due to pressure-driven ionic currents inside a three- dimensional nanoslit are obtained theoretically and numerically by finite element solution of governing equations, i.e., Poisson-Nernst-Planck, Ampere, and Navier-Stokes equations. The transport governing equations in this study are non-dimensionalized by Debye screening length, and discretized in a two dimensional finite length nanoslit. The magnetic field components have opposite signs above and below the nanoslit due to opposite directions of the Amperian closed path. Within the nanoslit the non-uniformity of ionic currents resulted in non-uniform magnetic fields however outside the nanoslit, magnetic fields remain relatively constant, independent of the distance from a sufficiently long and wide nanoslit. It is anticipated that non-invasive ionic/streaming current measurements can be conducted by external magnetic fields readouts

in sufficiently long and wide nanoslits. For instance, to estimate electrical properties (zeta potential) of solid-liquid interface, and to accurately sequence DNA and biomolecules.

A Review of Ionic-Liquid Electrospray Propulsion and Related Electrokinetic Phenomena

Authors

Mr. Louis Perna - Accion Systems, Inc

Prof. Paulo Lozano - MIT

Abstract

The formation of conical menisci in conductive liquids is an electrohydrodynamic phenomenon first studied by G.I. Taylor in detail in the early twentieth century. Electrosprays are sources of charged particles produced by these liquid structures. Subsequent studies led to the development of applications in chemical and biological instrumentation, micro- and macroscale manufacturing, and rocket propulsion. Fluid and material properties, system geometry, and electrical and mechanical stresses all play a role in determining the stability, repeatability, efficiency, and makeup of the electrospray emission.

Advancements in electrospray sources for space vehicle propulsion have been dominated over the last decade by the investigation and use of ionic liquids as highly-conductive, vacuum-stable propellants. Electrokinetic phenomena must be taken into consideration both at and upstream of the emission site in order to understand and predict source behavior and in order to design for reliability and performance. A review is provided of the electrospray phenomenon, historical work and applications, and recent developments specific to ionic-liquid ion-electrospray emission with a focus on electrokinetic phenomena and related challenges. Of interest are electrochemical stability, electro-osmosis, and interfacial double layer development and depletion dynamics in the propellant storage, flow, and emission elements of electrospray propulsion devices.

Single charging events on colloidal particles in a nonpolar liquid with surfactant

Authors

Prof. Filip Beunis - Ghent University

Dr. Caspar Schreuer - Ghent University

Mr. Bavo Robben - Ghent University

Prof. Filip Strubbe - Ghent University

Prof. Kristiaan Neyts - Ghent University

Abstract

Electrical charging of colloidal particles in nonpolar liquids due to surfactant additives is investigated intensively, motivated by its importance in a variety of applications. Most methods rely on average electrophoretic mobility measurements of many particles, which provide only indirect information on the charging mechanism. In the present work, we present a method that allows us to obtain direct information on the charging mechanism, by measuring the charge fluctuations on individual particles with a precision higher than the elementary charge using optical trapping electrophoresis.

We demonstrate the capabilities of the method by studying the influence of added surfactant OLOA 11000 on the charging of single colloidal PMMA particles in dodecane. The particle charge and the frequency of charging events are investigated both below and above the critical micelle concentration (CMC) and with or without applying a DC offset voltage. It is found that at least two separate charging mechanisms are present below the critical micelle concentration. One mechanism is a process where the particle is stripped from negatively charged ionic molecules. An increase in the charging frequency with increased surfactant concentration suggests a second mechanism that involves single surfactant molecules. Above the CMC, neutral inverse micelles can also be involved in the charging process.

We also observe that the particles gain positive charge during the experiments. The rate of this charging phenomenon is proportional to the amplitude of the applied electric field and the charging stops when the voltage is switched off. We propose a reaction mechanism where the particle sheds negatively charged ions, that accounts for the experimental observations of this electric field induced charging phenomenon.