RESEARCH SCHOLARS’ DAY
CELEBRATING RESEARCH BY CHE PG STUDENTS

NOVEMBER 4, 2018
VENUE: L-16, 9:00 AM - 6:00 PM

A ONE DAY SYMPOSIUM ON FRONTIER CHE RESEARCH IN

SENSORS AND NANOFABRICATION
CHEMICAL REACTION ENGINEERING
NANOSCIENCE AND NANOTECHNOLOGY
COMPLEX FUIDS AND FLOWS
THERMODYNAMICS
SOFT MATTER
... AND MANY MORE

C. V. Seshadri Memorial Distinguished Lecture by Dr. Rochish Thaokar, Professor, Department of Chemical Engineering, IIT Bombay on “Droplet levitation, breakup, emulsification and coalescence in electric fields”

Special lecture by Dr. Gurunath Ramanathan, Professor, Department of Chemistry, IIT Kanpur on “How to remain an ethical academician?”
# PROGRAM AT A GLANCE

## ChE Research Scholars’ Day
**4th November, 2018, IIT Kanpur**

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WELCOME TO CHE RESEARCH SCHOLARS' DAY, 2018

Inspired by the adage, “The important thing in science is not so much to obtain new facts as to discover new ways of thinking about them”, the Department of Chemical Engineering, IIT Kanpur organizes the one-day annual symposium simply entitled “Research Scholars’ Day” to celebrate and showcase the frontier chemical engineering research by its post-graduate students. Senior PhD students share their on-going research in the form of oral talks and poster presentations to fellow students, faculty, invited academicians and other attendees. In addition to valuable feedback and critique of their work, the occasion helps promote meaningful collaboration through increased awareness on the various on-going research activities in the department and also promotes strong student-faculty bonding. An eminent scientist from outside IITK is also invited to deliver a plenary talk as a highlight of the symposium. The occasion provides a unique platform for intellectual growth of the students through exchange of ideas, thoughts, vibes and inspirations in the stimulating and vibrant ambiance.
MESSAGE FROM HEAD

Dr. Animangsu Ghatak
Head
Chemical Engineering

The Department of Chemical Engineering at IIT Kanpur has established itself as one of the best destinations in the country for chemical engineering research and education. The faculty and students of the department carry out cutting-edge research in a wide spectrum of areas covering traditional chemical engineering and a range of inter-disciplinary subjects. The “Research Scholars’ Day” of the department provides a perfect opportunity to showcase the research work carried out by our post-graduate students, and also provides a platform for deliberations and discussions, both within the department as well as with the larger Institute community. The department is indeed very proud of the achievements and contributions made by our post-graduate students, and we are sure that the seminars will be exciting and thought-provoking. We welcome all of you to attend the symposium and participate in its proceedings. Further, the plenary lectures of the day will be the C V Seshadri distinguished lecture in chemical engineering for the year 2018 to be delivered by Dr. Rochish Thaokar of IIT Bombay and special lecture by Dr. Gurunath Ramanathan of IIT Kanpur.
The Department of Chemical Engineering at IIT Kanpur is among the nation's top ChE schools. We are endowed with highly distinguished and committed faculty, a vibrant graduate program attracting the nation’s best young researchers and a highly competitive undergraduate program. Our research portfolio encompasses fundamental and applied research in emerging and core areas of chemical engineering. It spans the frontier areas of sustainable process engineering, complex fluids and flows, energy and environment, nanoengineering and science and multi-scale molecular simulations. We also have strong research collaborations with the industry for solving design, control and optimization problems as well as involved problems related to interfacial phenomena, macromolecules and complex fluids. Our research is published in top-notch international journals and the training of our post-graduates is very rigorous, both in terms of breadth of courses studied as well as depth in the chosen area of research. Over the years, our faculty has published over 30 textbooks and research monographs and our students have gone on to become leaders in industry and academia.

Currently, we are 20 faculty members, who excel in diverse facets of cutting-edge chemical engineering research, ~75 highly sought after PhD research scholars, ~60 M Tech scholars and ~300 undergraduates students. The multifarious activities of the department are ably supported by eighteen technical/administrative support-staff members.

The department has been continually adapting and responding to the rapidly changing economic, social and technological scenario at the national and international levels. From modest beginnings as a fledgling undergraduate program in the early 1960s, ChE@IITK has grown into a unique blend of passionate research and pedagogical pursuits. If you share such a passion, do seriously consider joining us as a faculty or a student.

www.iitk.ac.in/che/
Rochish Thaokar joined IIT Bombay in 2005 and is currently professor in the department of chemical engineering. He obtained his B. Tech from LIT Nagpur, ME and PhD from IISc Bangalore, followed by a Postdoctoral stint at Max Planck Institute for Polymerforschung in Mainz, Germany. He also worked for a year in TRDDC Pune. His research interests include pattern formation in planar electrohydrodynamic systems, drop emulsification and coalescence using electric fields, capsule and vesicle electrohydrodynamics for dielectrophoresis and electroporation applications as well as droplet levitation and breakup in electric traps. He uses analytical theory, experimental methods and boundary integral calculations to understand electrohydrodynamics of soft matter.
Droplet levitation, breakup, emulsification and coalescence in electric fields

Electrohydrodynamics of aqueous droplet systems in non-conducting media such as air and insulating oils are encountered in quite a few applications. These include electrosprays, mass spectrometry and ion-traps, electro-emulsification of water in high viscosity oils and electrocoalescence in desalting of crude oils. It is well known that a spherical drop charged beyond its Rayleigh limit becomes unstable (when subjected to a small shape perturbation) and ejects a significant fraction of the original charge in the form of a jet. Our computations predict the charge loss in the Rayleigh breakup process wherein the drop is modelled as a perfect conductor. The extension of this model to include charge dynamics, which is typically ignored in the literature owing to the great difference in the conductivities of the droplet and the medium (air), highlights the importance of tangential stresses in formation of a jet and progeny droplets. Another problem where the fast but finite dynamics of charges in aqueous systems is important is the electrocoalescence of droplets under electric field. One of the major applications and successes of electrohydrodynamics is in the desalting process in refineries, where salt is removed from oil by destabilization of the water-in-oil emulsion using electrocoalescence. The physics of two droplets under electric field is complicated and yields surprises such as non-coalescence under strong fields. Moreover, quite non-intuitively, the mode of non-coalescence seems to depend upon the nature of oil and the conductivity of the aqueous droplets, indicating relevance of charge dynamics.
“HOW TO REMAIN AN ETHICAL ACADEMICIAN?”

Dr. Gurunath Ramanathan
Professor
Department of Chemistry
IIT Kanpur
ABSTRACTS:
ORAL PRESENTATIONS

DEPARTMENT OF CHEMICAL ENGINEERING, IITK
A simulation study of Ni₃Fe alloy using embedded atom potentials
Anil Mangla, Pankaj A. Apte, and Goutam Deo

A simulation study of Ni₃Fe alloy using embedded atom potentials. The alloys consisting of Nickel and iron as the primary components are used in a diverse range of applications. These include Maraging steels (15-20%Ni) used in engine components, the invar alloy (36%Ni 64%Fe) used in a variety of scientific instruments and Mu-metal alloy (77% Ni 16% Fe) which is used for shielding various instruments such as MRI, Hard disks, transformers from magnetic fields. Our focus in this work is on Ni₃Fe which has been found to catalyze several important reactions for example CO₂ methanation [1], CO methanation [2], cracking and reforming of CH₄[3]and in H₂ evolution reaction [4]. It shows higher reaction conversion compared to other pure Ni. Atomistic simulations can provide useful insights into the enhanced catalytic activity of the alloy. A detailed study of enhanced catalytic activity requires a semi-empirical potential that can reproduce the essential bulk and surface properties of the alloy. However, one needs an accurate interatomic potential to study the properties of the alloy. In the past few decades, a general class of potentials known as embedded atom (EAM) potentials has been found to successfully describe the properties of several metals and semi-metals. In these potentials, a subject atom is viewed as embedded in a pool of host electron with implicit self-consistent electronic density. The total energy of subject atom with host species is sum of embedded form of energy and pair interactions between atoms. However, in its original form, EAM potentials are isotropic in nature and hence could not describe metallic systems having covalent (directional) bonding. Specifically, potentials with the directional (anisotropic) components have been found to be essential in simulation of Fe-containing alloys including Ni₃Fe. In this work, we compare bulk properties of Ni₃Fe simulated using two EAM potentials (without the directional component) and an angular dependent EAM potential. These semi empirical models are developed using first principal calculations inputs and parameterized fitting is based upon experimental results and physical properties. We compare several properties such as lattice constants, elastic constants and XRD patterns against the experimental values. We discuss the possible reasons of deviations of the computed properties from experimental values. Further we also consider segregation of iron and nickel atoms in Ni₃Fe alloy surfaces of various orientations. The relevance of the segregation patterns observed to catalytic activities [5] is also discussed. References: 1. Dharmendra Pandey, Goutam Deo, J. Ind. Eng. Chem., 33 (2016), pp. 99-107. 2. Kuiwei Yang, Minhua Zhang, Yingzhe ,Int. J. Hydrogen Energy, 42 (2017), pp. 914-927 3. Koustuv Ray, Siddhartha Sengupta, Goutam Deo, Fuel Process. Technol., 156 (2017), pp. 195-203 4. R. Solmaz, G. Kardas, Electrochem. Acta, 54 (2009), pp. 3726-3734 5. Anil Mangla, Goutam Deo, Pankaj A.Apte, Comp. Material Science, 153(2018), pp. 449-460.
A linear stability analysis of pipe Poiseuille flow of an Oldroyd-B fluid has been carried out to investigate the interplay among fluid inertia, elasticity and the ratio of solvent viscosity to the solution viscosity. The stability has been analyzed for axisymmetric perturbations using pseudospectral and shooting methods. The system is linearly unstable at the Reynolds numbers relatively lower than the values for which the transition to turbulence is observed for the Newtonian pipe flows. The system has been analyzed for the vast ranges of the wavelengths, Reynolds number, elasticity number and the ratio of solvent to the solution viscosity. In the limit of low elasticity the fluctuations are found to be close to the axis of the pipe, hence we refer this unstable mode as ‘centre mode’. This unstable mode stabilizes in the UCM limit (absence of solvent). Various scalings that are followed by threshold and critical parameters have been discussed. Comparisons of the present results with the experimental results in the existing literature have been made to establish a theoretical evidence that this instability should serve as a preliminary stage in the exploration of the dynamical pathway to the elasto-inertial turbulence in the polymer solutions.
Increasing atmospheric carbon dioxide and sulfur dioxide emissions from combustion of fossil fuels, such as coal and oil, are considered a globally alarming environmental issue. Hence, the quest for an immediate solution for sequestration and storage of carbon dioxide and sulfur dioxide is warranted. Recently, amine and ionic liquid-based absorption processes have attracted widespread attention to capturing these gases, but this process passes several disadvantages such as severe corrosion, highly energy intensive, and low contact area. [1] One viable alternative is adsorption technology, which is recognized to be attractive to replace current absorption technology. Therefore, development of novel porous carbon-based materials has become one of the hot areas due to their extensive applications in gas storage and separation. In this regard, first, we have modeled an experimentally observed 3-D porous structure of graphene sponge (GS) using molecular dynamics simulations (MD). [2] The initial structure is composed of randomly distributed graphene flakes and inclusion particles of variable dimensions following the lognormal distribution. MD simulations are performed using Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential to mimic the synthesis of 3-D graphene sponge.

Further, we have used this graphene sponge as an adsorbent to capture CO\textsubscript{2}/SO\textsubscript{2}. We have performed Grand Canonical Monte Carlo (GCMC) simulation to get adsorption isotherm and to examine selectivity for CO\textsubscript{2} and SO\textsubscript{2} in graphene sponge. Our simulation results show that graphene sponge obtained using smaller size inclusion particles have large uptake capacity at post-combustion conditions. We first tested pure component flue gas adsorption capacity in graphene sponge then we moved on for the more realistic ternary mixture (CO\textsubscript{2}/SO\textsubscript{2}/N\textsubscript{2}) of flue gas adsorption. Pure component adsorption results show that SO\textsubscript{2} adsorbs preferably over CO\textsubscript{2} and N\textsubscript{2}. At 1 bar, the extent of excess adsorption of SO\textsubscript{2} and CO\textsubscript{2} in GS of 10 Å pore size is found to be 13 mmol/g and 2.6 mmol/g, respectively. Upon increasing pore size to 20 Å excess amount decreases by 56 % and 58 % for SO\textsubscript{2} and CO\textsubscript{2}, respectively. In the case of a ternary mixture, we have found that adsorption follows the same order as in the pure component flue gas adsorption, but adsorption amount decreases significantly. Selectivity analysis of adsorption shows that adsorption selectivity of SO\textsubscript{2} over N\textsubscript{2} is highest followed by the selectivity of CO\textsubscript{2} over N\textsubscript{2} and SO\textsubscript{2} over CO\textsubscript{2}.

Thus, our results indicate that graphene sponge obtained using smaller size inclusion particles is a promising material for the treatment of flue gas at post-combustion conditions.
At the limit of stability of a supercooled tetrahedral liquid modeled by monatomic (mW) water potential, it was recently shown that relaxation occurs across a unique value of per particle potential energy, which corresponds to a dynamical (non-stationary) condition of Gibbs free energy function $G(T,P,N,E)$. In this work, we explore the inherent structure responsible for the formation of the amorphous states though such a mechanism of relation of mW liquid. We first identify 6-member boat and chair shaped rings using a criterion based on the internal dihedral angles. We then consider the stacking of the cubic diamond (10-atom cluster with 4 chair shaped rings) and hexagonal wurtzite (12-atom cluster with 3 boat and 2 chair shaped rings) units through a shared chair ring. We find that the local crystalline (tetrahedral) order is exhibited by the eclipsed bond particles of the laterally connected wurtzite units which are stacked from both side with the diamond units (DWD stacking). Increasingly longer range crystalline order is obtained as the number of stacked wurtzite layers increases: the particles shared by the stacked (laterally connected) wurtzite layers in DWWD shows longer range crystalline order. An even longer range crystalline order is exhibited by the eclipsed bond particles of the middle (laterally connected) wurtzite layer of DWWWD stacking. We find that cubic-hexagonal stacking occurs primarily in the form of DWD layers across the limit of stability. The local tetrahedral order of the purely cubic (Diamond) network particles (which are not shared with wurtzite units) deviates significantly from that of the hexagonal crystal. Nonetheless, the average length of the bond in the purely cubic network approaches that in the hexagonal crystal very closely. Thus a large increase in the purely cubic ice across the instability also leads to an increase in the crystalline order in the form of bond lengths. Our results are consistent with previous experimental and simulation studied which find a significant fraction of cubic ice along with cubic-hexagonal stacking layers in the deeply supercooled water.
Flow of a power-law fluid across an asymmetrically confined rotating cylinder
Pooja Thakur, Naveen Tiwari, and R.P. Chhabra

Fluid Flow past a rotating cylinder: Momentum and Heat transfer Characteristics. The study of the fluid flow across a rotating cylinder is of fundamental interest for several reasons like for flow control, lift enhancement, boundary layer control, etc. In addition, a rotating cylinder in non-Newtonian fluids also have a direct relevance in various industrial applications like calendering and sheet making process in polymer, paper making and the textile industries to the cylindrical cooling devices in the glass and plastics industries, etc. For such a flow, the kinematics of the flow is determined by both the bulk velocity and the angular velocity of the cylinder. Thus, for instance, the flow becomes asymmetric due to the cylinder rotation and the mixing increases which is desired for the above stated applications. Also, the flow field far away from the cylinder is, of course, influenced very little by its rotation. In view of such diverse possibilities, the present study has been performed for two conditions, first where rotating cylinder placed in a stream of bulk fluid i.e., no wall effects have been considered. In second, wall effects have been considered by placing the cylinder asymmetrically in a confined channel. For each case, the nonlinear field equations have been solved numerically using the finite element based solver Comsol Multiphysics (version 4.3a). In particular, the goal of this work is to study the momentum (streamlines, pressure coefficient, drag and lift coefficients and torque acting on rotating cylinder) and heat transfer (isotherms, local and average Nusselt number) characteristics for the flow of power-law fluids. The study have been conducted for high range of Reynolds number; 100 ≤ Re ≤ 500. Cylinder rotation delayed the transition from the steady flow to a periodic time-dependent regime. Thus, the critical conditions for flow to become time-dependent have been identified. In power-law fluids, effect of confinement and asymmetry position of the cylinder have also been identified for the range of conditions as follows: Reynolds number (10−3 ≤ Re ≤ 40), power-law index (0.3 ≤ n ≤ 1), blockage ratio (0.2 ≤ β ≤ 0.99) and asymmetry ratio (10−3 ≤ γ ≤ 1). In general, the moderate degree of cylinder confinement stabilizes the flow. At high Reynolds numbers, the stabilizing effect is outweighed by the shear-thinning behaviour of the fluid and the degree of symmetry and the flow field transits from the steady to time-dependent. The numerical results are supplemented by a lubrication approximation analysis relevant for the acute values of β and γ. The geometric and dynamic conditions for the validity of the lubrication approximation are also been generalized for power-law fluids.
Hydrodyanamic and constitutive instabilities in the flow of a shear-thinning viscoelastic fluid

Ramkarn Patne, G. Subramanian, and V. Shankar

Concentrated polymer solutions, melts and wormlike micellar solutions commonly encountered in processing industries exhibit strong shear thinning and viscoelastic properties. We study the linear stability of planar Couette, Poiseuille and Hagen-Poiseuille flows of a shear-thinning viscoelastic fluid using the White-Metzner (W-M) model, which incorporates both viscoelasticity and shear-thinning in a phenomenological manner. The analysis predicts the existence of an instability absent for a purely viscoelastic or shear-thinning fluids which is present only when the fluid is both shear-thinning and viscoelastic. We show that the same instability mechanism is operative in plane Couette flow, plane Poiseuille flow and pipe Poiseuille flows of W-M fluid. Our prediction is also consistent with instabilities observed experimentally in plane Poiseuille and Hagen-Poiseuille flows of concentrated polymer solutions. Further analysis in the constitutively unstable region reveals that the above instability is in fact continuation of the constitutive instability to the constitutively stable region. Thus, we establish for the first time a connection between constitutive and hydrodynamic instabilities.
Bi-metallic layered double hydroxide nanostructures for high-performance supercapacitor applications

Ankit Tyagi, and Raju Kumar Gupta

In recent times, the demand for portable electronic devices like mobile phones, cameras, and laptops, etc. is increasing day by day. Therefore, energy storage devices such as batteries and supercapacitors have significant importance because of their high energy density and high power density, respectively. Supercapacitor devices are gaining a great amount of attention because these use less toxic material, offer high power density, excellent electrochemical stability, a wide range of operating temperatures and durability. Facile fabrication of low-cost, efficient, stable, eco-friendly and earth-abundant electrode materials for supercapacitors is critical.

In the current study, we have studied bi-metallic layered double hydroxides materials because of their higher energy densities than carbon materials (graphene, CNT, activated carbon, etc.) and better redox behavior than transition metal oxides (MnO\textsubscript{2}, RuO\textsubscript{2}, etc.) which are commonly used for supercapacitor applications. Layered double hydroxide (LDH) is a new class of material having the general formula $[\text{M}^{2+} \text{M}^{3+}(\text{OH})_2]^x[A^{n^-},m\text{H}_2\text{O}]^{x-}$

[where M\textsuperscript{2+} and M\textsuperscript{3+} are the bivalent and trivalent metal cations and A\textsuperscript{n-} is the charge balancing anion of valence n];

$$x = \frac{\text{M}^{3+}}{\text{M}^{2+} + \text{M}^{3+}}$$

has shown enormous supercapacitive performance. Ni-V LDH was chosen because of the better redox behavior of Ni as well as higher conductivity of V. We have studied the effect of varying the ratio of Ni and V to optimize the supercapacitive performance of Ni-V LDH. Further, flexible hybrid supercapacitor device was fabricated through coating Ni-V LDH on Ni foam. Devices showed high energy density of ~30.6 W h kg\textsuperscript{-1} at a power density of 0.78 W kg\textsuperscript{-1}. In order to fabricate binder free flexible hybrid supercapacitors, Ni-V LDH was directly grown on flexible carbon cloth substrate (NVL@CC). Hybrid supercapacitor device based on NVL@CC//Activated carbon showed good energy density and could light 1.8 V red LED for 1 min. There is no degradation of device performance observed even after 5000 charge-discharge cycles.
Novel carbon-based nanomaterials in situ dispersed with metal nanoparticles for hydrogen production, storage and environmental remediation applications

Ashish Yadav, and Nishith Verma

Energy crisis and environmental pollution have currently emerged as the two major global challenges. Therefore, there are burgeoning efforts worldwide to find alternative energy sources. Hydrogen (H\textsubscript{2}) is considered to be alternative to fossil fuels because of its clean and renewable characteristics and large abundance. However, one of the main challenges associated with the practical usage of H\textsubscript{2} as a fuel is the development of a sustainable light weight on-board H\textsubscript{2} storage system. In regard to environmental remediation, there arises acute necessity to treat and recycle wastewater. Technically, this requires the efficient and cost effective catalysts for treating organic pollutants containing industrial wastewater effluents. The first study pertaining to the energy application describes the preparation of nickel (Ni) NP-containing microporous and graphitic carbon nanofibers (CNF)-based adsorbent for H\textsubscript{2} storage. The results revealed that the SBET of the materials controlled the storage capacity at cryogenic temperature. On the other hand, the positive synergistic effects of the graphitic CNFs and the metal (Ni) in the materials were clearly elucidated at elevated temperatures. The motivation behind the second study was to enhance the H\textsubscript{2} storage capacity and reduce the operating conditions of temperature and pressure which can render the H\textsubscript{2} storage process to be energy extensive. In this direction, a bimetallic configuration consisting of Ni and ceria (CeO\textsubscript{2}) NPs dispersed in microporous and graphitic CNF-ACF-based adsorbent was developed to efficiently store H\textsubscript{2} at 200 °C and 1 bar. The adsorbent was also completely regenerated at 300 °C and 1 bar. The third study focused on the energy application aspect pertaining to the development of an efficient electrode for H\textsubscript{2} production in microbial electrolyte cell (MEC). A Ni-graphene dispersed carbon film was prepared and the laser ablation technique was utilized for the fabrication of three dimensional (3D) micropillars on the carbon film. The MEC using the prepared electrodes produced H\textsubscript{2} at the rate of 4.22 ± 0.21 m\textsuperscript{3}/m\textsuperscript{3}-d. Thus, the prepared electrode offers a viable alternate to the noble metal-based electrodes used in MEC. The study pertaining to environmental remediation focused on the catalytic wet air oxidation (CWAO) technique used for the destruction of organic pollutants in wastewater. This study describes the preparation of iron (Fe) metal NPs-doped carbon microbeads (~0.5 mm) as the catalyst for the abatement of phenol, a model organic contaminant, from water by the CWAO technique. The CNFs were grown on carbon microbead via catalytic CVD technique, using acetylene as the carbon source. The results reveal an efficient remediation of the phenol-laden water. In view of the practical applications, the previous study was performed under flow conditions. The K-oxidant impregnated and CNF grown Cu NP-doped carbon beads of approximately 0.5 mm size were successfully synthesized as an efficient catalyst for the abatement of organic pollutants in wastewater. The developed catalyst and the process were also successfully tested against a high COD (~120,000 mg/L O\textsubscript{2}) containing industrial wastewater effluent and the results reveal almost complete COD reduction (> 99%).
Laminar-turbulent transition for the flow of polymer solutions through micro-tubes

Bidhan Chandra, V. Shankar, and Debopam Das

Experiments are performed to characterize laminar-turbulent transition for the flow of polymer solutions through micro-tubes of size ∼ 400mm using micro-PIV and dye stream visualization techniques. Using small diameter tubes enable us to probe high elasticity number. We observe that addition of small amounts of polymer (50ppm-100ppm) delays transition to turbulence as compared to a Newtonian fluid whereas addition of larger amounts of polymer (500ppm-800ppm) causes an early transition. Earlier studies relating to early transition for the flow of polymer solution through tubes was limited to larger tube diameter and the onset of transition was detected by the use of pressure measurements (Samanta et al., 2013). It is observed that addition of polymer decreases velocity fluctuations in the post-transition regime irrespective of the concentration of polymer added for polyacrylamide solutions which may be linked to the drag reduction phenomena. The phenomena was corroborated by using a different polymer of a different molecular weight. Transition Re observed in our experiments (by varying polymer concentration, with tubes of different diameters and by using two different polymers) shows a remarkable data collapse. Micro-PIV and dye stream visualization technique is used to track instabilities in the flow of Newtonian and polymer solutions through rigid and deformable micro-tubes. Relaxation time and viscosity is measured using a concentric and a cone and plate geometry of a Rheometer. Relaxation time is calculated using small amplitude oscillatory tests and viscosity is measured with increasing shear rate using flow sweep experiments. Micro-PIV (micro-particle image velocimetry) consists of a camera, a synchronizer, a microscope and a laser. Fluorescent micro-sized particles are dispersed in the test solution and the resulting solution is pumped through the prepared micro-tube (micro-tubes prepared using PDMS) with the help of a syringe pump. Tracking the displacement of the particles during the flow enable us to get velocity vectors in the micro-tube. Normalized standard deviation in velocity with time is calculated. A jump in the normalized standard deviation in velocity is considered as the onset of transition. Further a shift in the ratio of center-line peak to cross-sectional average velocity is considered as a signature of transition. Flattening of the parabolic velocity profile is further used as method to verify the onset of transition. Transition detected using micro-PIV is further verified using dye-stream visualization experiments. A thin line of dye is injected using a separate syringe pump into the flow. Reynolds number is increased in a step-wise manner and the breakage of the dye stream is considered as an indicator of transition. The break-up of the dye stream is recorded using a high speed camera and hence used to infer the onset of transition.
Effect of roughness on the conductivity of vacuum coated flexible paper electrodes
Gaurav Rawal, and Animangsu Ghatak

Flexible conducting materials are required for design and fabrication for a host of applications, e.g. flexible displays, flexible electronic sensors, wearable electronics, flexible transistors, solar cells, a variety of energy storage and energy harvesting devices and so on. The process of making these flexible electrodes involve coating or printing a conducting layer on a flexible substrate, e.g. a polymeric membrane, crosslinked elastomer, paper, fabric of a different kind and so on. A large number of coating methods have been developed which include solution processing, thermal evaporation, electrodeposition, in-situ deposition of metal nanoparticles and nanowires, ink-based coating and printing, physical vapour deposition (PVD), vacuum filtration, sintering and solvothermal coating, etc. Although many of these conducting plates are made on a flexible, yet rough substrate like a paper via vacuum deposition of a metal, the exact role of the roughness of these substrates vis-à-vis the effective conductivity of the coating is not understood. Importantly, how precisely the roughness or the 3D porous structure of the paper surface affects the microscopic grain structure of the metal coating has not been examined in detail. With the objective of elucidating the coupled effect of substrate roughness and surface energy on the conductivity of the paper electrode, we have used six different papers commonly available in the market for coating them with copper layers of varying thickness. The effect of paper surface roughness on the deposited copper layer stability, copper grain size and shape was assessed. Papers with different roughness and surface energy were coated, and the microstructure of the coated layer was analysed using SEM. Our results show that the conductivity depends on grain density and size which in turn depends on the roughness of the paper. The macrostructural effect of roughness and the increase of resistance with roughness has been established. In contrast, we show that there is a sublevel structural effect, the shape and size of grains deposited that effects the resistance. For a smooth surface, the grains that constitute the coating appear spherical, however, turns ellipsoidal as the substrate roughness and heterogeneity is increased; ellipsoidal grains result in higher packing efficiency leading to higher conductivity. The role of grain micro-structures based on shape and size distribution of grains is demonstrated and a novel theoretical model, which relates the shape and size distribution of deposited grains to the effective packing efficiency and hence the conductance is developed. The percolation limit is investigated in terms of size, shape, and packing of the particles. We have also examined the change in resistance with the number of copper-coating layers, number of folds and repeated bending of the pipe.
Resistance to fracture of a soft elastic gel by a sharp object like a hypodermic syringe needle depends upon the macroscopic geometry of the tool. While this topic has been examined to some detail, somewhat less explored issue is the effect of vibration on gel fracture, particularly the coupled effect of geometry and vibration. The topic is however important as it is encountered in many natural systems: for example, the hierarchical structure of mosquito proboscis and its vibratory motion, both are thought to influence the puncturing load. In this context we have carried out displacement controlled fracture of a soft gel using a syringe needle while also subjecting the gel to longitudinal vibration at controlled frequency and amplitude. During puncturing of gel with a syringe needle, fracture occurs in two different modes: a primary crack propagates ahead of the needle tip whereas a secondary crack emanates radially away from it; these cracks do not propagate simultaneously but alternatively, suggesting that one propagates at the expense of the other. Occurrence of the secondary crack implies that larger load is required to drive the primary crack which in the context of tissue puncture increases the pain. Here, we show that occurrence of the secondary crack can be controlled by introducing relative vibration between the needle and the gel, which in turn reduces the maximum puncture load required to drive the primary crack and arrests also the occurrence of side cracks thereby allowing stress concentration to attain critical level ahead of the needle tip for fracture to occur. The puncturing load diminishes for increase in amplitude of vibration and the extent of decrease depends upon of the structure of the puncturing tool and modulus of the gel. We have also presented a scaling analysis to rationalize this dependence. The difference in the maximum puncturing load, for a given vibration with respect to the no vibration condition is scale as . These results throw light on fracture in many natural systems involving soft materials where the vibratory motion of the puncturing tool as also observed with mosquito proboscis and also relevant for understanding fracture in similar other contexts, for example, cutting a block of soft material using a thin object like a slender cylindrical rod, or a knife.
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Mass and charge transport aspects in the electrochemical detection of heavy metal ions in aqueous solutions conjugated polymer based sensors

Kusumita Dutta, and Siddhartha Panda

Selectivities of electrochemical sensors to interfering ions have been characterized by reduction of the height of the signal peak which require a large number of experiments, and by the selectivity coefficient techniques which have limitations. In this work, using conducting polymer based sensors and utilizing the calculations of barrier widths at different concentrations, the experimental interference behaviour of various ions (Na\(^+\), K\(^+\), Mg\(^{2+}\), Sr\(^{2+}\), Mn\(^{2+}\), Al\(^{3+}\), As\(^{5+}\), Zn\(^{2+}\), Fe\(^{2+}\), Fe\(^{3+}\), Pb\(^{2+}\), Cu\(^{2+}\), Cr\(^{6+}\)) with respect to cadmium ion were successfully correlated. This technique demonstrated for the first time for interference studies in sensors, overcomes limitations of earlier techniques and could be used as a predictor for the extent of interference for different sensor systems. Utilizing cyclic voltammetry and electrochemical impedance techniques, barrier widths for the systems were calculated. Based on the ratio of the barrier width of cadmium ion with the interferant to that of only cadmium ion in buffer solution, a scale was developed which correlated with the results obtained from the conventional peak reduction method. The utility of this work is that with a smaller number of experiments, the interference behaviour of ions can be predicted for a given system. In the next phase of our work, this BW technique was benchmarked with the peak reduction technique for its claim of usage and to develop a scale of interference with a higher resolution. In this work, utilizing the BW technique we report the analysis based on Cd\(^{2+}\) concentrations spanning two orders of magnitude and interfering ions (Al\(^{3+}\) (less interfering), Fe\(^{2+}\) (moderately interfering) and Cr\(^{6+}\) (heavily interfering)) also spanning two orders of magnitude. The sensitivity parameters were benchmarked thereby validating BW technique. Adsorption isotherms were constructed for each case and −ΔGads values were evaluated. A correlation obtained from the sensitivity parameters from the BW and PR techniques and −ΔGads yielded an interference scale with a resolution higher than that of the scale obtained by the PR technique or the BW technique. In order to approach lower detection limit, it was required to study on the material aspect of the substrate. To increase the active surface area of the copolymer film, an additive was incorporated into its backbone. In this case the thickness of the film and the amount of an additive were varied to improve the LOD. LOD for cadmium was achieved to 2 ppb while high tolerance level of cadmium was achieved from less interfering and moderately interfering ions. Response surface analysis was done, based on which a suitable thickness for the film was identified with desired amount of additive which was able to detect cadmium till 800 ppt and magnificent tolerance level was achieved for highly interfering ion. In case of copolymer the tolerance ratio was 1:1 (Cd\(^{2+}\): Cr\(^{6+}\)) which improved to 1:8 (Cd\(^{2+}\):Cr\(^{6+}\)). The mechanism of variation of the sensing process with respect to film thickness and amount of additive was explained by BW technique as well as a new technique Dispersion frequency technique (DF technique) which also explained the interference phenomena equally well.
ABSTRACTS:
POSTER PRESENTATIONS
The study presents a numerical investigation of hydrodynamic characteristics of Bingham plastic fluids by a rotating cylinder placed in a rectangular T-channel junction for the purpose of controlling flow and understanding the insight of flow mechanism. The governing differential equations have been solved in the laminar flow regime employing the finite element method over wide ranges of Reynolds number ($10^{-2} \leq Re \leq 40$), Bingham number ($10^{-2} \leq Bn \leq 20$) and rotational velocity ($-0.5 \leq \alpha \leq 0.5$) where $\alpha$ is the cylinder circumferential velocity normalized by free stream velocity. In particular, the new extensive results are presented in terms of streamline patterns, shape and size of yielded/unyielded regions in the vicinity of T-channel, drag and lift coefficients, flow split ratio (i.e., the ratio of main branch flow rate to the side branch) and torque. As expected, yield-stress fluid stabilizes the flow by suppressing the recirculation zones while Reynolds number destabilizes the flow. The cylinder rotation affects the flow dynamics significantly and the torque required to rotate the cylinder decreases with an increase in rotational velocity.
Organometal halide hybrid perovskites have recently emerged as one of the most promising material for optoelectronic applications. Their exceptional characteristic properties such as high carrier mobility, tunable band gap, long diffusion length, ease of fabrication, etc render them a remarkable material for variety of optoelectronic applications in photovoltaics, light emitting diodes (LEDs), photodetectors, LASER and more. Dewetting of thin polymer films have been explored for creating micropatterns and hierarchical nano/micro-structures. In this work, we report dewetting of composite thin films of methyl ammonium lead iodide (MALI) perovskite and polystyrene (PS) to form microdroplets of polymer containing MALI. Ordered micropatterns can be obtained by either prepatterning of films prior to dewetting or prepaaterning of substrate. PS can be subsequently removed by dissolving in organic solvents to leave MALI micropaaterns. Such micropatterns can be utilized to fabricate array of microLEDs or a photodector with micron-sized pixels for improved sensitivity.
Copper and graphene oxide dispersed carbon film used as an electrode for the electro-oxidation of diclofenac
Arun Kumar, and Nishith Verma

The increasing concentrations of diclofenac (DCF), a widely used anti-inflammatory drug, in water bodies is an emerging concern because of its persistent characteristics. Conventional remediation techniques are inefficient in treating such pollutants. Therefore, there is an urgent requirement of advance treatment technologies. In the present study, a novel copper-graphene oxide (Cu-GO) dispersed phenol polymeric film was synthesized. The polymeric matrix in situ dispersed with Cu-GO was carbonized and reduced to synthesize self-standing electrode. The prepared materials were characterized for their various physicochemical properties. The Cu-rGO electrode was used in the electro-oxidation of aqueous DCF. The electrochemical behaviour was assessed by performing cyclic voltammetry (CV). The electrode could generate a high oxidative faradic current response, which was sufficient to presume that synthesized electrode had good electrochemical behaviour. Approximately, 100 % COD reduction was recorded within 3 h when 2 V constant potential was applied for 200 ppm of DCF. The dual role of Cu-rGO was presented as: Cu showed extremely high over potential for oxygen evolution. The oxidation peak in CV at -0.5 V vs. Ag/AgCl indicated direct oxidation of diclofenac. High non-faradic current of 400 mA observed at positive potential indicated the indirect oxidation of the pollutant.
Mitochondria are the powerhouse of mammalian cells. They produce energy to maintain various functionalities of all the vital cellular processes and remain mobile so as to distribute energy throughout the cell. Since, mitochondria are the key regulators of cell death, targeting mitochondria to kill cancer cells is a promising approach for chemotherapy based cancer treatment. Nanoparticles have been used in the past for intracellular delivery of therapeutic agents. However, targeting mitochondria is very challenging as the carrier needs to overcome not only cell membrane but also barriers offered by outer and inner mitochondrial membranes. Various mitochondria targeting moieties are generally employed to direct nanoparticles specifically to mitochondria. In the present work, we have developed a new class of nanoparticles using polydimethylsiloxane (PDMS) and found them to possess inherent tendency to get selectively localized inside mitochondria without any mitochondrial targeting moieties. Our in vitro results further demonstrate efficient delivery of doxorubicin, a model anticancer drug via PDMS nanoparticles in human cervical cancer (HeLa) cell lines. In vivo evaluation of the nanoparticles in mice model is currently under process of investigation.
Defect state modulation of TiO$_2$ for degradation of emerging pharmaceutical pollutants
Deepanshu Aggarwal, Prasanjit Kar, Pratyush Jain, and Raju K. Gupta

The removal of emerging pollutants in water using simple TiO$_2$ via photocatalysis technique is very much limited because of its wide band gap (~3.2 eV) and lack of visible light absorption ability. Here, we have investigated defect state modulation of TiO$_2$ for degradation of emerging pollutant i.e. Antipyrine in water under visible light irradiation. Antipyrine, which is commonly used for medication to get relief from pain, congestion and swelling is found to be an emerging pollutant in water. We have used a simple hydrothermal technique for the synthesis of TiO$_2$ microspheres (average diameter ~2 μm). We further employed chemical reduction method for the formation of defective TiO$_2$ microspheres using reducing agent under inert atmosphere for different time interval (3 h, 5 h and 8 h). The extent of defects on TiO$_2$ microspheres has significantly shown impact on optical properties and photocatalytic activity. Defected TiO$_2$ microspheres were utilized for photocatalytic degradation of antipyrine under visible light illumination. Improved photocatalytic activity for the defect TiO$_2$ samples was observed due to reduction in band gap as well as incorporation of Ti$^{3+}$ which acts as a trap state and results in reduction in the electron–hole recombination.
In the present work, the effect of time-dependent pulsatile flow on momentum and heat transfer characteristics of an unconfined sphere submerged in an incompressible power-law fluid have been investigated numerically using a finite element based solver. Flow and thermal characteristics are examined over the following range of conditions: Reynolds number \(5 \leq \text{Re} \leq 120\), Prandtl number \(0.7 \leq \text{Pr} \leq 100\), power-law index \(0.3 \leq n \leq 1.5\), Strouhal number \(\pi/4 \leq S \leq \pi\) and amplitude of pulsation \(0 \leq A \leq 0.8\). The flow is assumed to be laminar and axisymmetric. The induced flow pulsatility is observed to further complicate the kinematics leading to the formation of unsteady viscous eddies on the surface of the sphere. As expected, the flow and thermal fields evolve in a time-periodic fashion. The vortex on the surface of the sphere grows in size during the deceleration phase of the pulsatile cycle and vice versa. The frequency \(S\) and amplitude of pulsations \(A\) play a pivotal role. The pulsatile flow is observed to enhance the heat transfer rate of shear thinning fluids by a maximum 30\% (at \(\text{Re} = 120, \text{Pr} = 100\)) over that of the non-pulsatile flow under identical conditions.
We study temperature induced phase change of a block copolymer Pluronic F127 having a concentration in a range: 20-35 wt %. While this temperature dependent phase change visually appears like a liquid-soft solid transition, there is a debate regarding precise microstructure of the soft solid state. In this work, we carry out frequency sweep at various temperatures on F127 solution. We observe that irrespective of the concentration in the explored range, an aqueous solution of F127 shows all the rheological characteristic features of sol–gel–glass transition. Such behavior suggests the transition of a liquid sample to a space spanning percolated network, whose rheological characteristic is increase in tan δ with frequency, followed by a glassy transition as characterized by a peak in tan δ. Interestingly, the maxima in tan δ shifts to lower temperatures with an increase in frequency, which illustrates the rate dependence of glass transition. The glass transition temperature is observed to decrease with increase in the concentration of F127. The glass transition behavior is also observed at higher temperature during gel melting. Dynamic light scattering has been employed to study the evolution of micellar radius with temperature in F127 solution. Finally, based on the rheological studies we construct a phase diagram.
Shear banding and delayed yielding in thixotropic yield stress fluids
Mayank Agarwal, Lakshmi Kushwahaa, V.Shankar, and Yogesh M. Joshi

The objective of current work is to analyze delayed yielding and associated shear banding in creep in thixotropic yield stress fluids by carrying out experiments and simulations. Creep experiments have been performed on Ludox gel for stresses above and below the yield stress. In thixotropic materials yielding behaviour depends on applied stress, state of the material and the time over which the stress is applied. For some thixotropic materials it has been observed that a prolonged application of creep, wherein even though shear rate decreases with time initially, strain shows a sudden increase eventually. We observe an increase in yield stress as we increase the waiting time after shear rejuvenation. The time scale at which yielding starts in material decreases with the difference between the stress and the yield stress as the power law. Then we study the transient response of the Couette flow subjected to step stress using fluidity model proposed by Coussot et al., 2002. We observe that the inclusion of inertia has significant influence on the existence of the transient as well as steady state shear bands. We also observe that, sufficiently aged samples (non-zero waiting time) show the presence of delayed yielding.
The effect of adding $O_2$ to the Dry Reforming of Methane reaction over Ni/MgAl$_2$O$_4$ and Ni/Al$_2$O$_3$

Neeraj Koshta, Puneet Kumar Chaudhary, and Goutam Deo

Dry reforming of methane (DRM) is an environmentally friendly reaction that utilizes CO$_2$ and methane to produce synthesis gas. Unfortunately, coking and catalyst deactivation frequently occur when the reaction is carried out over supported nickel catalysts. To overcome these drawbacks O$_2$ is added. In the present study the DRM reaction is carried out in a packed bed reactor at 600 and 750°C and at 1 atm using nickel supported on MgAl$_2$O$_4$ and Al$_2$O$_3$ catalysts. The catalysts were synthesized using the incipient-wetness impregnation method. Furthermore, the fresh and spent catalysts were characterized by H$_2$-TPR, SEM, TGA, CHNSO, and XRD. For an equimolar inlet of CO$_2$:CH$_4$ and in the presence and absence of O$_2$ the reaction was analyzed. At 600°C the CH$_4$ conversion and carbon deposited on the catalyst was more than that at 750°C. Additionally, the carbon deposited on Ni/MgAl$_2$O$_4$ was more than carbon deposited on Ni/Al$_2$O$_3$. Upon adding 2.6 mol % O$_2$ to the feed, the amount of carbon deposited was reduced at both temperatures. Furthermore, the CH$_4$ conversion and H$_2$/CO ratio increases in the presence of oxygen. Thus, including limited amounts of O$_2$ to CO$_2$ + CH$_4$ was beneficial for the reaction in several ways.
Emulsions, being widely used in a host of practical applications, mostly involves generation of drops of a specific morphology, e.g., simple microspheres and cylinders to complex core-shell, Janus droplets and so on, depending on particular application. But many other applications demand reversible alteration between these different morphologies of complex emulsion droplets, which, in general, is triggered by the solvent pH, temperature, surfactant, in essence, parameters which alter the interfacial energy between different phases. Here we show that the morphology of dispersed double emulsion droplets can change also because of confinement of the emulsion. In particular, we have generated core-shell and Janus droplets using silicone oil, paraffin oil in aqueous solution of Agarose as three immiscible phases. In bulk emulsion, core-shell drops appear with paraffin oil at core and silicone oil at the shell. However, the morphology of oil droplets changes to Janus when the emulsion is confined between two parallel plates.
Electropolymerized acryl amide nano film grown over in situ Ni nanoparticle-dispersed graphene oxide and N-doped phenolic polymer composite: A non-enzymatic recognition element-based glucose sensor electrode

Pallab K Bairagi, and Nishith Verma

Development of non-enzymatic electrochemical sensors for the measurement of glucose, a diabetes biomarker is of prime interest over the last decade because of low chemical stability of enzyme-based electrode. In this study we have developed reduced graphene oxide in situ dispersed with Ni-nanoparticles and N-doped phenolic polymer composite (Ni rGO/P) as the working electrode for the glucose biosensor. Poly (acryl amide) (PAA) nanofilm was successfully grown on the surface of the Ni_rGO/P composite using electropolymerization for the first time. The PAA molecule was used for the glucose recognition and measurement also for the first time. The prepared sensor electrode (PAA_Ni_rGO/P) materials were characterized using different physico-chemical methods by the SEM, XRD, RAMAN, XPS. Different electrochemical techniques viz. electrochemical impedance spectroscopy, cyclic voltammetry, etc. were used for measuring electrochemical properties e.g. impedance, electrochemical active area and response time of PAA_Ni_rGO/P. Tested with differential pulse voltammetry, PAA_Ni_rGO/P showed remarkable linearity over 0.03 – 250 mgdL-1 concentration with high reproducibility and found to have negligible effect on response in the presence of the interfering biomolecules such as uric acid, urea, ascorbic acid, cholesterol etc. PAA_Ni_rGO/P was also applied successfully to the clinical samples (RSD<6%).
A novel scheme towards improving the consistency of bead-spring models of polymer chains in dilute solutions

Praphul Kumar, and Indranil Saha Dalal

Traditionally polymer chains have been modelled by beads connected by a set of springs. A finer model for a polymer chain is to represent each Kuhn step by rods, or nearly inextensible Fraenkel springs. Although the latter is expected to be closer to the true representation of the chain, the coarser bead-spring models are assumed to be sufficiently accurate to model the chain dynamics. We perform detailed Brownian dynamics simulations, which prove that the results from these different representations agree only qualitatively. Quantitatively, the predictions depend on the “level” of coarse-graining i.e. the number of springs selected to model the chain. In this work, we introduce a novel correction to the conventional bead-spring method by allowing the mass to be distributed along the springs, instead of being concentrated at the bead centre. All results obtained with this modification agree remarkably well with those obtained from the finer bead-rod models.
Capacitors having high energy density are urgently needed for the development of commercial, consumer, and military systems to fulfil the demand of low cost, compact, and efficient electrical devices. The advantages of using polymers are high breakdown strength while the nanofillers have high dielectric constant. However, incorporating nanofillers in the polymer matrix results into the formation of defects and voids surrounding the nanofiller interface, thereby reducing the breakdown strength remarkably. Thus, the interfacial modulation of the nanofillers is necessary to improve the dielectric properties. In this work, titanium dioxide (TiO$_2$) nanoparticles (NPs) are surface modified with barium titanate (BT) as well as TiO$_2$ followed by polydopamine shell to serve as nanofiller while polyvinylestene fluoride (PVDF) has been used as polymer matrix. Here, core as well as outer TiO$_2$ shell act as capacitor plates due to its high conductivity while BT acts as dielectric. Thus, each NP acts as an individual capacitor. The modification of the nanofillers helps in tailoring and improving the interface and dielectric performance of the capacitor. Further, it helps in homogenising the electric field and restricts the charge movement across the film as compared to the pristine TiO$_2$/PVDF capacitors.
Flows through helical channels are important for a host of scientific and engineering applications. The curvature and torsion of the helices have been revealed to stimulate secondary flow in addition to the primary axial flow, which enhances passive in-plane mixing between fluid streams. Most of these studies involve a single spiral with circular cross-section, which in essence is symmetric. The coupled effect of asymmetry of cross-section, curvature and torsion of channel would affect the flow profile inside such tubes which are yet to be explored and understood. In this perspective, here we have presented the analysis of fluid flow at low Reynolds number inside a novel triple helical channel which consists of three helical flow paths conjoined along their contour length leading to single multihelical flow geometry. We have performed both micro particle image velocimetry (µ- PIV) and 3D simulation in FLUENT of flow of a Newtonian fluid through such flow system, the results from simulation corroborates reasonably well with experimentally determined flow profiles. Our analysis also shows that in case of triple helical channels, number of vortices increases with the helix angle.
Soft glassy materials are highly viscous materials, that are thermodynamically out of equilibrium, which undergo structural evolution as a function of time. The process of structural evolution causes decrease in free energy, a process known as physical aging. The application of deformation field on the other hand causes structural breakdown that, in principle, increases free energy, a process known as rejuvenation. Many soft glassy materials, under application of constant strain subsequent to shear melting, often demonstrate residual stress that do not decay over the practical timescales. Interestingly with increase in intensity of shear melting some materials show increase in the magnitude of residual stresses while other materials show decrease in magnitude of residual stress. In this work, we employ a multi-mode structural kinetic model that employs Sprigg’s relaxation time spectra. We observe that the diverse experimental observations can be captured by varying the width of relaxation time spectrum.
Perovskite solar cells have become an attractive light-absorber system with a rapid improvement of cell efficiencies from less than 4% in 2009 to a certified 22.7% in 2018. The low conductivity of TiO$_2$ poses obstacle in its efficiency enhancement. We present our results on Ta doped TiO$_2$ (Ta-TiO$_2$) compact layer as an ETL, having device structure FTO/compact-TiO$_2$/CH$_3$NH$_3$PbI$_3$/P$_3$HT/Ag. Ta doping in TiO$_2$ was confirmed through XRD, XPS and Raman spectroscopy. Charge carrier dynamics studies on Ta-TiO$_2$ thin films PL and KPFM shows that shift in the Fermi level along with improved conductivity of Ta-TiO$_2$ results in enhancement of the short circuit current and fill factor of the devices. Further, Ta doping of 3.0% led to a 40% improvement in the overall efficiency as compared with undoped TiO$_2$. Power conversion efficiency of ~9% was obtained for the perovskite solar cell devices using Ta doped compact TiO$_2$. 
A Study of the Dynamics of Human Pedestrians Using Experiments and Simulations in the Indian Context
Satyendra Pandey, Amullya Kale, Ishan Prashant, and Indranil Saha Dalal

Management of big crowd, especially when well-populated places are connected together, is extremely challenging. The objective of this study is to optimally design such public spaces, using well known scientific tools, to minimize the risk of stampede-like disasters. This would require the effective “interaction potential” between pedestrians. Towards this goal, we performed experiments with pedestrians in various scenarios. Our results show a severe mismatch of predicted dynamics of pedestrians, when earlier models were used. This is not entirely surprising, since those are developed in the context of western countries, whose population densities are typically one order of magnitude lower than that of India. We developed a correction to the existing models, which, to our belief, adds the effects on the dynamics due to human intelligence. With this correction, the predictions matched the experimental data exceptionally well. We are currently in the process of studying the motions in more complicated scenarios.
Stability analysis of the flow of Newtonian fluid in a deformable channel with an unrestrained boundary
Shraddha Mandloi, and V. Shankar

Linear stability analysis of the plane Poiseuille flow of a Newtonian fluid past a deformable linear-elastic solid channel for an unrestrained top boundary is performed in this work. Recently, the flow in a rectangular deformable channel made of a polyacrylamide gel with an unrestrained top wall was examined in an experimental study by S.S. Srinivas and V. Kumaran (J. Fluid Mech., 822, 267–306 (2017)), to determine the effects of the soft wall on transition and turbulence. In order to understand the effect of the “unrestrained” boundary on the dynamics of the high-Reynolds number instabilities, we performed a numerical linear stability analysis of the system. We observed that for both wall-mode (\( \text{Re} \sim \Sigma^{(3/4)} \)) and inviscid mode instability (\( \text{Re} \sim \Sigma^{(1/2)} \)), the presence of unrestrained boundary destabilizes the flow. We also performed an asymptotic analysis for the wall modes and observed that the results are in good agreement with the complete numerical solution of the governing stability equations. We further showed that there is no effect of the lower solid layer with the restrained boundary on the critical Reynolds number and hence the instability is only affected by the \( H \) and \( \Gamma \) values of the top solid layer with the unrestrained boundary.
In spite of therapeutic and diagnostic advances, the 5-year survival rate for oral squamous cell carcinoma (OSCC) remains at about 50%. One of the major factors accounting for the poor outcome of patients with OSCC is that a great proportion of oral cancers are diagnosed at advanced stages and, therefore, treated late. Given the fact that current diagnostic method is falling short to detect the disease early enough, we propose a paper based biosensor to detect oral cancer biomarkers from saliva by using impedance spectroscopy technique. In this work we have identified two antigens namely Epidemic Growth Factor (EGF) and Tumor Protein (p53), presence of which has been widely identified with oral cancer. We have fabricated a whatman filter paper based biosensor which can detect EGF and p53 by using a technique called Electrochemical Impedance Spectroscopy (EIS). EIS gives us a clear picture of the interfacial phenomena in terms of charge transfer resistance (Rct). The paper based biosensor thus fabricated proves to be highly sensitive, selective and having a very low detection limit. We feel devices such as the one proposed here can be extremely helpful as a point of care device (POC)