3rd MELBOURNE INDIA POSTGRADUATE PROGRAM AND MELBOURNE INDIA POSTGRADUATE ACADEMY CONFERENCE (MIPPAC 2022)

DATE: 3rd – 4th February 2022

BY

THE UNIVERSITY OF MELBOURNE

With Partnering Institutes

IIT Kanpur, IIT Kharagpur, IIT Madras, IISC Bangalore & IISER Tirupati

DIRECTOR'S MESSAGE

A/Prof
Meenakshi Arora
Director,
MIPP & MIPA

Professor
Muthupandian
Ashokkumar
Deputy Director,
MIPP & MIPA

We are pleased to extend a very warm welcome to you all to the 3 rd MIPP/MIPA Conference (MIPPAC 2022) during 3-4 Feb 2022. We are especially delighted to welcome participation from our two new partners Indian Institute of Science (IISc) Bangalore and Indian Institute of Science Education and Research (IISER) Tirupati.

The conference will look a bit different this year as it's a virtual event due to ongoing pandemic restricting overseas travel and large gatherings. But we believe the conference will provide a unique opportunity to larger cohort of interested students and academics from all partner institutions to participate and engage in a range of professional development and technical sessions. In addition to technical session, where our young researchers will share their work, the conference also offers two professional development panels with our recent graduates as well as with well-established industry professionals in Australia and in India. These panel members will share not only their academic experiences during and after their PhD journey, but also some important insights into finding a fulfilling career in a different country and maintaining work-life balance. MIPPAC presents a unique opportunity that it brings together researchers and academics from a wide array of scientific interests. This richness of ideas provides a very enriching environment for cross fertilisation of ideas, explore multi-disciplinary collaborations

We are particularly excited about the engagement and ongoing support from the leaders of University of Melbourne and all the partner institutions. Under their leadership, MIPP/MIPA have grown year to year even during the pandemic. Special thanks are also due to the organising committee members and the session chairs, for the time, energy and thought that they have invested in organizing the program. This conference would not be possible without their generous support.

Most of all, we thank you all for enriching the conference by your participation, contributions and scientific debates. The last two years have been very challenging for everyone and as we begin 2022, it's time to reflect at what we have achieved despite the challenges imposed on us by COVID-19. We hope 2022 will bring new opportunities and collaborations with more outstanding and enthusiastic graduate researchers (GRs) and world class academics and this will surely drive our bilateral research excellence. MIPPAC 2022 will provide a perfect platform for networking and initiating new collaborations.

We hope you will enjoy the conference, renew old friendships, make new friends, get new ideas, and above all, have a good time.

ABOUT MIPA/MIPP

The Melbourne India Postgraduate Program (MIPP) and the Melbourne India Postgraduate Academy (MIPA) are joint initiatives of The University of Melbourne and a selected group of India's elite research universities: IIT Kanpur, IIT Kharagpur, IIT Madras, IISc Bangalore & IISER Tirupati. MIPP and MIPA provides graduate researchers opportunities to work with joint supervisors from the University of Melbourne and one of the program's Indian partners. The program offers PhD living stipend and fee remission scholarships and associated support for researcher exchanges and cooperation.

By enabling students from India and Australia to undertake jointly developed research of the highest quality, the program provides them with the opportunity to contribute to the development of educational, cultural and industry links between both countries. The students get access to research facilities and expertise at both institutions. In addition, all the participating students join as a member of the exclusive MIPP/A cohort at University of Melbourne and receive mentoring from staff as well as a wide network of IIT alumni groups settled in Victoria.

Our GRs benefit from undertaking an international joint-training experience in an elite research community where they will learn to adapt to new cultural and research environments; be mentored and supported by field experts; have access to research facilities and equipment at two institutions; and additionally have the opportunity to establish strong international networks to promote research exchange and high quality publications.

Participating academics are granted rare opportunities to develop and sustain research collaborations that draw from a pool of complementary skills, world class expertise and infrastructure, establishing a more competitive and impactful platform from which to address the critical scientific questions and global challenges of our time.

Like the previous edition MIPPAC-2017 & MIPPAC-2019, MIPPAC-2022 conference will provide an intellectually stimulating environment for researchers from UoM and partnering institutions to strengthen existing collaborations and foster new partnerships.

PARTNER INSTITUTES

INDIAN INSTITUTE OF TECHNOLOGY KANPUR (IITK)

IIT-Kanpur was established as the fourth IIT in India in 1959. It is located 15 km west of Kanpur City in North India and occupies a land close to 420 hectares. It has about 350 faculty members and about 6400 (50% undergraduate and postgraduate each) students. Most research areas in Engineering and Science are represented at IITK. It is known for its research in Engineering and Science.

INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR (IIT KGP)

IIT Kharagpur is the first Indian Institute of Technology established in India. It was established in 1951 in Kharagpur, in the eastern part of India. IIT Kharagpur has 19 academic departments, 8 multidisciplinary centers/schools, 13 schools of excellence and central research facilities. IIT Kgp is perhaps the largest and the most diversified among the IITs

INDIAN INSTITUTE OF TECHNOLOGY MADRAS (IITM)

IIT-M was formally inaugurated in 1959 in Chennai with the assistance of the German Government as the 3rd IIT in India. It is a residential institute with nearly 550 academic staff, 8000 students and 1250 administrative and supporting staff and is a self-contained campus located in a land of about 250 hectares. The Institute has sixteen academic departments and some advanced research centers in various disciplines of engineering and pure sciences, with nearly 100 laboratories. It has strong relationships with industry and its staff and students are of very high quality.

Indian Institute of Science Bangalore (IISc Bangalore)

IISc is the top ranked research institution in India. It was conceived as a 'Research Institute' or 'University of Research' by Jamsetji Nusserwanji Tata in the final years of the 19th century and was established in May 1909. The Institute offers a variety of Master's degree programs in Engineering, an integrated PhD (post-B.Sc.) program in Sciences, and PhD programs in a wide spectrum of disciplines in science and engineering. In addition, many national research facilities are housed at the Institute. The research laboratories at the Institute are extremely well equipped and the library and computational facilities at the Institute are amongst the best in India.

Indian Institutes of Science Education and Research Tirupati (IISER) Tirupati

The Government of India, through the Ministry of Education, has established seven Indian Institutes of Science Education and Research (IISERs).The IISERs represent a unique initiative in India where teaching and education are integrated with state-of-the-art research, nurturing both curiosity and creativity in an intellectually vibrant atmosphere of research. Each IISER is an autonomous institution awarding its own Masters and Doctoral degrees.

BOOK OF ABSTRACTS

PRESENTING AUTHORS AND ABSTRACT LINKS*:

*Click on the links to go to the abstract of the presenting author

PARTNERING INSTITUTE : IIT KANPUR	
1	***Mr. Ankit Bhadouriya:*** New understanding of Open-ocean Deep Convection in the Southern Ocean
2	***Mr. Mehdi Alam:*** Soft-rigid bonded granular mixes: Particle Scale Study to Field Predictions
3	***Mr. Shreshtha Gupta:*** CO Modelling of Flame-Wall interaction
4	***Mr. Sourav Ghosh:*** Microstructure Evolution of Cobalt-based Superalloy: A Multiscale Study
5	***Mr. Subhajit Chakraborty:*** A Customized Microspectroscopic Arrangement for Imaging High Refractive Index Media with TIRFM Approach
PARTNERING INSTITUTE : IISc BANGALORE	
6	***Ms. Chesta:*** Photo-rechargeable Zinc-ion Batteries
PARTNERING INSTITUTE : IIT KHARAGPUR	
7	***Mr. Amrish Kumar Padmakumar:*** Ultrasound Assisted Controlled Radical Polymerization
8	***Mr. Anirban Ghosh:*** Quench Dynamical studies of a finite extended SSH Model
9	***Mr. Arunjunai R. S. Santha Kumar:*** Light induced RAFT Polymerisation of acrylamides; Effect of ionic liquids
10	***Mr. Biswajit Palar:*** Lake Records from northern and eastern India and model runs to understand monsoon variability during the last millenium
11	***Mr. Chinglen Tensubam:*** Global and regional (Southern Ocean) time series analysis of Chl-a concentration and study of its correlation with physical processes
12	***Mr. Joydeep Baral:*** Structure-function insight into the two-component NHEJ DNA repair system of Mycobacterium tuberculosis
13	***Mr. Joydip Mondal:*** Investigation of chemical and physical effects from acoustic bubble(s) in partially-degassed liquid
14	***Mr. Mayank Bhasin:*** Simulation and Modelling of Organic PV Nanoparticles
15	***Mr. Pawan Kumar:*** Contact Angle Hysteresis on Surfaces with Random Topology

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PROGRAM SCHEDULE

Venue: Zoom
[https://unimelb.zoom.us/j/4866738776?pwd=dnhiUzV3NHZ1SnVKVHA5K3Y0ZUdDUT09]

DAY 1: 3rd Feb 2022 [THURSDAY]

Plenary Session: 02.00 PM - 03.10 PM AEDT | 8.30 AM - 9.40 AM IST

TIME AEDT [IST]		Speakers	Chair
From	To		
2.00 PM [8.30 AM]	2.05 PM [8.35 AM]	Introduction to MIPP/A & Welcome to MIPPAC 2022: ***Session Chair***	Ms. Snigdha Sarita Mohapatra
2.05 PM [8.35 AM]	2.15 PM [8.45 AM]	Welcome Note: MIPA Director ***Dr. Meenakshi Arora***	
2.15 PM [8.45 AM]	2.25 PM [8.55 AM]	***Prof. Justin Zobel***, Pro-Vice-Chancellor Graduate & International Research, The University of Melbourne	
2.25 PM [8.55 AM]	2.35 PM [9.05 AM]	***Prof. Mark Cassidy***, Dean of Faculty of Engineering and IT , The University of Melbourne	
2.35 PM [9.05 AM]	2.45 PM [9.15 AM]	***Prof. Moira O'Bryan***, Dean of the Faculty of Science, The University of Melbourne	
2.45 PM [9.15 AM]	2.55 PM [9.25 AM]	***Prof. Vijayamohanan Pillai***, Dean (R&D), IISER Tirupati	
2.55 PM [9.25 AM]	3.05 PM [9.35 AM]	***Prof. Jayanta Mukhopadhyay***, Dean Outreach, IIT Kharagpur	
3.05 PM [9.35 AM]	3.10 PM [9.40 AM]	***Prof Michael Wesley,*** Deputy Vice-Chancellor International	

Technical Session - I : 03.10 PM - 04.40 PM AEDT | 9.40 AM - 11.10 AM IST

TIME AEDT [IST]		Topic and Presenter	Chair
From	To		
3.10 PM [9.40 AM]	3.25 PM [9.55 AM]	***Mr. Ankit Bhadouriya:*** New understanding of Open-ocean Deep Convection in the Southern Ocean	Mr. Dibbendu Roy
3.25 PM [9.55 AM]	3.40 PM [10.10 AM]	***Mr. Mehdi Alam:*** Soft-rigid bonded granular mixes: Particle Scale Study to Field Predictions	
3.40 PM [10.10 AM]	3.55 PM [10.25 AM]	***Mr. Shreshtha Gupta:*** CO modeling of Flame-Wall Interaction	

3.55 PM [10.25 AM]	4.10 PM [10.40 AM]	***Mr. Sourav Ghosh:*** Microstructure Evolution of Cobalt-based Superalloy: A Multiscale Study	
4.10 PM [10.40 AM]	4.25 PM [10.55 AM]	***Mr. Subhajit Chakraborty:*** A Customized Microspectroscopic Arrangement for Imaging High Refractive Index Media with TIRFM Approach	
4.25 PM [10.55 AM]	4.40 PM [11.10 AM]	***Ms. Chesta:*** Photo-rechargeable Zinc-ion Batteries	

Session Break | Change of Chair: 04.40 PM - 04.45 PM AEDT | 11.10 AM - 11.15 AM

Professional Development Session: 4.45 PM - 5.45 PM AEDT | 11.15 AM - 12.15 PM IST

Topic: So, you completed your PhD - What's next? A panel discussion highlighting career opportunities after PhD

TIME AEDT [IST]		Panel Members	Chair
From	To		
4.45 PM [11.15 AM]	5.45 PM [12.15 AM]	[A] **A/Prof. Kathryn Mumford** [Chemical Engineering, The University of Melbourne] [B] **Prof. Suresh Bhargava** [PVC International, RMIT] [C] **A/Prof. M. K. Tiwari** [School of Water Resources, IIT Kgp] [D]**Dr. S. Akalya [**Food Processing Business Incubation Centre, National Institute of Food Technology, Entrepreneurship and Management (NIFTEM) - Thanjavur]	Ms. Noor E Karishma Shaik & Mr. Ankit Bhadouriya

Session Break | Change of Chair: 05.45 PM - 06.00 PM AEDT | 12.15 PM - 12.30 PM IST

Technical Session - II : 06.00 PM - 07.30 PM AEDT |12.30 PM - 02.00 PM IST

TIME AEDT [IST]		Topic and Presenter	Chair
From	To		
6.00 PM [12.30 PM]	6.15 PM [12.45 PM}	***Mr. Amrish Kumar Padmakumar:*** Ultrasound-Assisted Controlled Radical Polymerization	Mr. Shrestha Kumar Gupta
6.15 PM [12.45 PM]	6.30 PM [01.00 PM]	***Mr. Anirban Ghosh:*** Quench Dynamical studies of a finite extended SSH Model	
6.30 PM [01.00 PM]	6.45 PM [01.15 PM]	***Mr. Arunjunai R. S. Santha Kumar:*** Light-induced RAFT Polymerisation of acrylamides; Effect of ionic liquids	
6.45 PM [01.15 PM]	7.00 PM [01.30 PM]	***Mr. Biswajit Palar:*** Lake Records from northern and eastern India and model runs to understand monsoon variability during the last millenium	
7.00 PM [01.30 PM]	7.15 PM [01.45 PM]	***Mr. Chinglen Tensubam:*** Global and regional (Southern Ocean) time series analysis of Chl-a concentration and study of its correlation with physical processes	
7.15 PM [01.45 PM]	7.30 Pm [02.00 PM]	***SESSION ENDS | DAY - 1 CLOSURE***	

DAY 2: 4th Feb 2022 [FRIDAY]

Plenary Session: 02.00 PM - 03.00 PM AEDT | 8.30 AM - 9.40 AM IST

TIME AEDT [IST]		Speakers	Chair
From	To		
2.00 PM [8.30 AM]	2.10 PM [8.40 AM]	Welcome to MIPPAC 2022 Day 2 : ***Session Chairs***	Mr. Sourav Ghosh & Mr. Dibbendu Roy
2.10 PM [8.40 AM]	2.20 PM [8.50 AM]	Welcome Note: MIPA Director ***Prof. Muthupandian Ashokkumar***	
2.20 PM [8.50 AM]	2.30 PM [9.00 AM]	***Prof. Yogesh M. Joshi***, Dean of International Relations, IIT Kanpur	
2.30 PM [9.00 AM]	2.40 PM [9.10 AM]	***A/Prof. Praveen Kumar***, Chair of International Relations, IISC Bangalore	
2.40 PM [9.10 AM]	2.50 PM [9.20 AM]	***Prof. Raghunathan Rengaswamy***, Dean Global Engagement, IIT Madras	
2.50 PM [9.20 AM]	3.00 PM [9.30 AM]	***Prof. Shanton Chang***, Associate Dean International, Faculty of Engineering and IT	

Session Break | Chair Allotment : 03.00 PM - 03.10 PM AEDT | 9.30 AM - 9.40 AM

Technical Session - I : 03.10 PM - 04.40 PM AEDT | 9.40 AM - 11.10 AM IST

TIME AEDT [IST]		Topic and Presenter	Chair
From	To		
3.10 PM [9.40 AM]	3.25 PM [9.55 AM]	***Mr. Joydeep Baral:*** Structure-function insight into the two-component NHEJ DNA repair system of Mycobacterium tuberculosis	Mr. Sourav Ghosh
3.25 PM [9.55 AM]	3.40 PM [10.10 AM]	***Mr. Joydip Mondal:*** Investigation of chemical and physical effects from acoustic bubble(s) in partially-degassed liquid	
3.40 PM [10.10 AM]	3.55 PM [10.25 AM]	***Mr. Mayank Bhasin:*** Simulation and Modeling of Organic PV Nanoparticles	
3.55 PM [10.25 AM]	4.10 PM [10.40 AM]	***Mr. Pawan Kumar:*** Contact Angle Hysteresis on Surfaces with Random Topology	
4.10 PM [10.40 AM]	4.25 PM [10.55 AM]	***Mr. Soumendu Sarkar:*** Petrogenesis of coeval lamproites and kimberlites from the Wajrakarur field, Southern India: new insights from olivine compositions	
4.25 PM [10.55 AM]	4.40 PM [11.10 AM]	***Mr. Subhrasankha Dey:*** Traffic state estimation using crowd-sourced data without road sensors	

Session Break | Change of Chair: 04.40 PM - 04.45 PM AEDT | 11.10 AM - 11.15 AM

Professional Development Session: 4.45 PM - 5.45 PM AEDT | 11.15 AM - 12.15 PM IST

Topic: So, you completed your PhD - What's next? A panel discussion highlighting career opportunities after PhD

TIME AEDT [IST]		Panel Members	Chair
From	To		
4.45 PM [11.15 AM]	5.45 PM [12.15 AM]	[A] ***Dr. Krishna Chandran*** [Demonstrator/Tutor, UoM] [B] ***Dr. Mukesh Soni*** [Engineering Problem Solver] [C] ***Dr. Punit Rathore*** [Assistant Prof. IISC Bangalore] [D] ***Dr. Salil Goel*** [Assistant Prof. IIT Kanpur]	Ms. Snigdha Sarita Mohapatra & Mr. Shrestha Gupta

Session Break | Change of Chair: 05.45 PM - 06.00 PM AEDT | 12.15 PM - 12.30 PM IST

Technical Session - II: 06.00 PM - 07.30 PM AEDT |12.30 PM - 02.15 PM IST

TIME AEDT [IST]		Topic and Presenter	Chair
From	To		
6.00 PM [12.30 PM]	6.15 PM [12.45 PM}	***Mr. Abhishek Mondal:*** [Yet to Receive]	Mr. Shrestha Gupta
6.15 PM [12.45 PM]	6.30 PM [01.00 PM]	***Mr. Dibbendu Roy*** : Resource Allocation Policies for 5G/6G Applications in Access Networks with Optimization and AI	
6.30 PM [01.00 PM]	6.45Pm [01.15 PM]	***Ms. Snigdha Sarita Mohapatra*** : Integrated Urban Water Balance Model for Developing Countries	
6.45 PM [01.15 PM]	7.00 PM [01.30 PM]	***Mr. Ananth S M:*** Increasing efficiency of high-lift turbine blades with roughness and riblets	
7.00 PM [01.30 PM]	7.15 PM [01.45 PM]	***Ms. Padma Naveena Ganapam***: Structural and functional changes at the knee after anterior cruciate ligament reconstruction	
7.15 PM [01.45 PM]	7.30 Pm [02.00 PM]	***Mr. Srivathsan***: Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study	
7.30 PM [02.00 PM]	7.45 PM [02.15 PM]	***SESSION ENDS | MIPPAC 2022 CLOSURE***	

16	***Mr. Soumendu Sarkar:*** Petrogenesis of coeval lamproites and kimberlites from the Wajrakarur field, Southern India: new insights from olivine compositions
17	***Mr. Subhrasankha Dey:*** Traffic state estimation using crowd-sourced data without road sensors
18	***Mr. Abhishek Mondal:*** [Yet to Receive]
19	***Mr. Dibbendu Roy*** : Resource Allocation Policies for 5G/6G Applications in Access Networks with Optimization and AI
20	***Ms. Snigdha Sarita Mohapatra*** : Integrated Urban Water Balance Model for Developing Countries
PARTNERING INSTITUTE : IIT MADRAS	
21	***Mr. Ananth S M:*** Increasing efficiency of high-lift turbine blades with roughness and riblets
22	***Ms. Padma Naveena Ganapam***: Structural and functional changes at the knee after anterior cruciate ligament reconstruction
23	***Mr. Srivathsan***: Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study

New understanding of Open-ocean Deep Convection in the Southern Ocean

Ankit Bhadouriya[1, 2], Dr. Bishakhdatta Gayen[1], Prof. Joe Klewicky[1], A/Prof. Rakesh Mathpal[2]
Department of Mechanical Engineering, UoM[1]
Department of Aerospace Engineering, IIT Kanpur[2]

Abstract

Ocean circulation, which consists of a wide range of length and temporal scales, controls global heat, nutrient and carbon budget, affecting climate, weather, and ocean biology. Ocean circulation is primarily driven by buoyancy (differential heating and cooling in low and high latitudes, respectively) and mechanical (wind, tide, etc.) forcing. Especially in the Southern Ocean, surrounding Antarctica, buoyancy-driven mechanism gets prominent under the sea-ice and cold atmosphare. Antarctic Bottom Water is generated by the consequence of deep convection of heavy surface waters, due to extensive loss of buoyancy, that further moves down, flows northwards, and fills all major ocean basins, feeding a global thermohaline oceanic conveyor belt. Beneath the sea-ice convective instabilities help to ventilate enough heat flux through the pycnocline, creating vast open water areas within the sea-ice zone. These open areas in sea ice, also known as polynyas, can then expose surface water to frigid cold weather leading to sustained open-ocean deep convection. However, the mechanism of polynyas still lacks knowledge on its initial cause and its impact on a global climate.

Large-scale ocean and climate models are primary tools to study these processes; however, they are unable to capture small-scale turbulent convective cells resulting in inaccurate estimation of upper-ocean heat ventilation and circulation. Our study aims to investigate the open-ocean deep convections over Maud Rise, a seamount in the Weddell Sea, using both observational Argo float data and Large Eddy Simulation. We analyze the role of small-scale turbulent structures and mixing on the onset of polynya dynamics, their dominant role in heat transport and local ventilation.

References

[1] Campbell, E.C., Wilson, E.A., Moore, G.K., Riser, S.C., Brayton, C.E., Mazloff, M.R. and Talley, L.D., 2019. Nature, 570(7761), pp.319-325.
[2] Cheon, W.G. and Gordon, A.L., 2019. Scientific reports, 9(1), pp.1-9.
[3] Marshall, J. and Schott, F., 1999. Reviews of geophysics, 37(1), pp.1-64.

Keyword
Convection, Ocean circulation, Polynyas

Soft-rigid bonded granular mixes: Particle scale study to field predictions

Mehdi Alam[1], Dr. Arghya Das[2], A/Prof Mahdi Miri Disfani[3]
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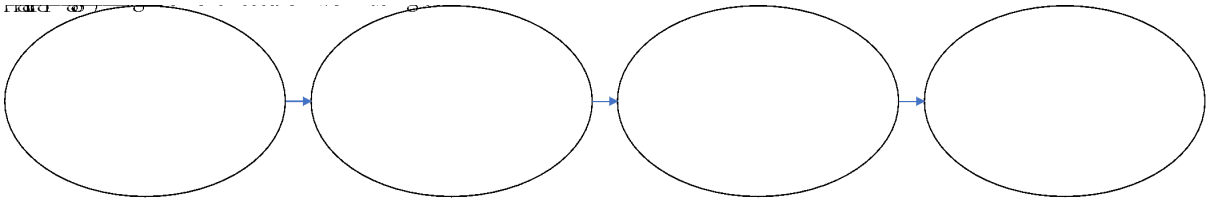
Department of Civil Engineering, IIT Kanpur[2]
Department of Infrastructure Engineering, The University of Melbourne[3]

Abstract

In the recent past, the research on the utilization of tyre and plastic chips (soft materials) as soil (granular materials) strengthening material is limited to laboratory-scale experiments and related numerical modelling. However, these works are carried out without accounting for the particle scale mechanisms and their utilization in robust field scale numerical modelling. Therefore, the conventional approach needs repetitive experiments for every mix prepared with different soft-rigid granular mixtures. Hence widespread use of such combinations has been discouraged. The present study tries to develop a generalized approach, subdivided into four parts: experiment and imaging, build the images in DEM, prediction of behaviour, and real-world application. The brief aims and objectives are shown in the flowchart in Fig 1.



References

[1] Asadi M, Thoeni K, Mahboubi A. An experimental and numerical study on the compressive behavior of sand-rubber particle mixtures. *Computers and Geotechnics*. 2018;104:185-195. doi:10.1016/j.compgeo.2018.08.006

[2] Lee JS, Dodds J, Santamarina JC. Behavior of Rigid-Soft Particle Mixtures. doi:10.1061/ASCE0899-1561200719:2179

[3] Guo N, Zhao J. A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media. *International Journal for Numerical Methods in Engineering*. 2014;99(11):789-818. doi:10.1002/NME.4702

Keyword

Soft-rigid mixes, DEM modelling, X-ray tomography

CO Modelling of Flame-Wall Interaction

Shreshtha Gupta[1,2], Mohsen Talei[1], Robert L. Gordon[1], Vaibhav K. Arghode[2]
Department of Mechanical Engineering, The University of Melbourne, Parkville, Victoria 3010[1]
Department of Aerospace Engineering, Indian Institute of Technology Kanpur, U.P. 208016[2]

Abstract
Flame-wall interaction (FWI) commonly occurs in gas turbine combustors and internal combustion engines. This phenomenon can lead to formation of pollutant emissions such as carbon monoxide (CO) when fossil fuels are used for combustion. This is because FWI impacts the transport mechanisms of CO in the near-wall region and can therefore result in unoxidized CO at the combustor exit. This work numerically examines the FWI phenomenon using Direct Numerical Simulations (DNSs) in order to develop accurate predictive models for locally produced CO concentrations. In this talk, the capability of Large Eddy Simulation (LES) sub-grid scale models in predicting CO species will be assessed for a premixed flame interacting with a relatively cold wall. Lookup tables for CO based on the temperature and a progress variable are found to be a promising approach for non-adiabatic CO modelling. A significant increase of the flame displacement speed as well as a large variation across different iso-values of the progress variable is observed. The results suggest that in the context of Flame Surface Density (FSD) based LES models, the entire flame front displacement speed term, $\overline{\rho S_d |\nabla c|}$ needs to be modelled, rather than just the wrinkling factor [1].

References

[1] Shreshtha K. Gupta, Rahul Palulli, Mohsen Talei, Robert L. Gordon, and Vaibhav K. Arghode. "CO modelling of premixed head-on quenching flame in the context of Large-Eddy Simulation." International Journal of Heat and Fluid Flow 93 (2022): 108895.hn and L. J. Sham, Phys. Rev., 1965, 20, 23175-23194.

Microstructure Evolution of Cobalt-based Superalloy: A Multiscale Study

Sourav Ghosh[1,2], Rajdip Mukherjee[1], Christian Brandl[2]
Department of Materials Science and Engineering, IIT Kanpur[1]
Department of Mechanical Engineering, The University of Melbourne[2]

Abstract

Superalloys are high temperature application alloys with a combination of mechanical strength and resistance to surface degradation. They are widely being used for their applications in gas turbines, coal conversion plants, and chemical process industries, and for other specialized applications requiring heat and corrosion resistance [1]. Microstructure evolution of Co-based super alloys are largely dependent on the coarsening kinetics of Ɣ'-phase precipitates in the gamma-phase matrix in Co-based super alloys. Gibbs-Thompson effect and LSW [2] (Lifshitz Slyozov Wagner) theory helps in better understanding of coarsening kinetics. Phase-field method is a simulation method based on diffuse interface approach, which is applicable to microstructural evolution and interfacial reaction in mesoscopic length scale. The key component of the phase-field method is the total free energy of the system which includes bulk free energy, interfacial free energy and elastic strain energy. The input parameters into the the phase-field model can be extracted from the molecular dynamics (MD) (nanoscale) simulation, calculation of phase diagram (CALPHAD) and first principle density function theory (DFT) calculation; where bulk free energy can be extracted from CALPHAD integration, intrface energy from MD and elastic eenrgy from DFT calculation. Our presentation will be on the development of phase-field model to study precipitate coarsening behaviour of Co-Al-W, a Co-based super alloy using a diffuse interface approach. Our future work will include atomistic and phase-field simulations to predict a parameter space to optimise morphology, volume fraction and size distribution of second phase particles to achieve desired properties.

References

[1] Roger C. Reed, The Superalloys Fundamentals and Applications, Cambridge University Press (2009), pp. 1-5

[2] A.M. Jokisaari, S.S. Naghavi , C. Wolverton, P.W. Voorhees, O.G. Heinonen, Predicting The Morphologies of Ɣ-Precipitates in Cobalt-based Superalloys, Acta Materialia, Volume 141, (2017) pp. 273-284

Keyword

Superalloys, Microstructure evolution, Phase-field

A Customized Microspectroscopic Arrangement for Imaging High Refractive Index Media with TIRFM Approach

Subhajit Chakraborty[1,2,3] , Yang Xu[2,3] , Ann Roberts[3,4] , Debabrata Goswami[1] and Trevor A. Smith[2,3]
Centre for Lasers & Photonics, IIT Kanpur, Kanpur, India [1]
School of Chemistry, University of Melbourne, Australia [2]
ARC Centre of Excellence in Exciton Science [3]
School of Physics, University of Melbourne, Australia [4]

Abstract
Total Internal Reflection Fluorescence Microscopy (TIRFM) enables us to investigate the interfacial tomography of the imaging object through the evanescent wave excitation [1]. The sharply decaying evanescent field is a consequence of the total internal reflection of the incident beam at the interface, which depends strongly on the refractive indices of the media constituting the interface [2]. A major difficulty arises when the refractive index of the object is higher than the incident substrate medium. The total internal reflection of the incident light is now no longer possible, and consequently, the evanescent wave excitation is also absent. We propose a customized microspectroscopic arrangement where imaging of the sample is possible even if its refractive index is higher than the incident substrate medium. The system is further optimized to increase its microscopic capabilities and enhance image quality.

References
[1] Axelrod, D., 2008. Total internal reflection fluorescence microscopy. Methods in cell biology, 89, pp.169-221.

[2] Hecht, E., 2002. Optics, 5e. Pearson Education India.

Keyword
Optics, Microscopy, TIRFM

Photo-rechargeable Zinc-Ion Batteries

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Abstract

Solar energy has been considered as one of the most promising, effective, and emission-free renewable energy resources to meet the global energy demands. However, due to the intermittent and fluctuating nature of solar energy, it requires to integrate batteries for energy storage along with solar panels. This extra electronics introduces energy losses and increases the overall cost. Photo-rechargeable batteries are a promising alternative to meet the energy demands using solar energy. It involves the use of a photocathode which both harvests and stores energy and hence reduces the extra electronics. Transition metal phosphotrichalcogenides have gained significant attention as 2D layered materials because of their tunable properties. They have the general formula MPX_3 where M is transition metal, P is phosphorus and X is S or Se chalcogen. These materials possess strong intralayer and weak interlayer forces which allows easy exfoliation of the material into different layers and hence tunable band gap. Due to this structural diversity, MPX_3 materials possess attractive electric and magnetic properties. Hence, they are promising materials to be studied for their optoelectronic as well as energy storage application. Aqueous zinc-ion batteries are potential energy storage devices due to their low cost, intrinsic safety, high gravimetric energy density and environmental friendliness. In this talk, preliminary studies carried out to investigate the use of transition metal phosphotrichalcogenide as a photocathode material for photo-rechargeable Zinc-ion batteries will be discussed.

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Keywords

Photo-rechargeable, Zinc-ion batteries, Transition metal triphosphochalcogenide

Ultrasound Assisted Controlled Radical Polymerization

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Polymers have significantly replaced metals in various sectors such as the aerospace, automotive, electronics, energy industries, etc. as they have the advantage of the greater design freedom, significant weight reductions, and improved performance. The recent development of controlled radical polymerization (CRP) leads to the synthesis of many well-defined architectures with predictable molecular weights [1]. Traditionally, thermally labile initiators (typically azo-containing compounds like AIBN) or redox-active transition metal catalysts have been employed to activate radical polymerization, leading to issues with product contamination and safety concerns, particularly in high-value applications such as food, consumer goods and healthcare. Ultrasound-assisted RAFT polymerization in aqueous media is a novel initiator-free, "green" polymerization technique [2]. Here, radicals produced ultrasonically would spread homogeneously throughout the reaction mixture. Under ultrasonic environment, the radical species are generated because of vaporization of liquid molecules into cavitational bubbles leading to their growth and subsequent spontaneous collapse, which in turn creates localized heat and pressure that degrades the water into its radical species such as hydroxyl radicals and hydrogen atoms. Employing this approach, we aim to remove the requirement for an exogenous radical initiator in aqueous controlled polymerizations. In addition, the living character of the polymer chains are studied to assess the capability to produce polymers with specific architectures such as star polymers, block co-polymers, etc and as well as to understand the chain extension properties under ultrasonic cavitation [3].

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Keywords
Ultrasound, Controlled Radical Polymerization, RAFT

Quench Dynamical studies of a finite extended SSH Model

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Abstract:

Some 1D chains can host topological phases that are characterized by the presence of edge states and a topological invariant like a non-zero winding number. An example of such a system is an SSH model which has staggered hopping amplitudes leading to two sublattices and it can host two edge states[1]. Recently there has been some very interesting studies on quench dynamics of topological models revealing some rich non-equilibrium properties. These studies can reveal information such as preservation of a topological phase, the robustness of the system, transport in non-equilibrium conditions, nature of topological phase etc[2][3]. We have performed quench dynamical studies on an extended SSH model. In the extended SSH model, long-range hopping up to 4^{th} nearest-neighbour hopping is introduced and it is confirmed that this model could have states of higher winding numbers i.e., winding numbers greater than one. We have used winding number diagrams to mark the topological phase of the system for the various parameter settings. We have then introduced and illustrated the concept of the path of winding number transition for two sets of initial and final winding number states. Next, we have studied the effect of the path of winding number transition on the quench dynamics of the edge states and we have shown a strong dependence of quench dynamics on the path chosen for winding number transition. We have then studied the size dependence of the quench dynamics and have found an interesting pattern. We have then explained the quench dynamics using the energy band diagrams for paths and transport of the edge state probability wave density making use of the light cone diagrams.

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Keywords: quench dynamics, topological phase, robustness.

Light induced RAFT Polymerisation of acrylamides; Effect of ionic liquids

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Abstract:

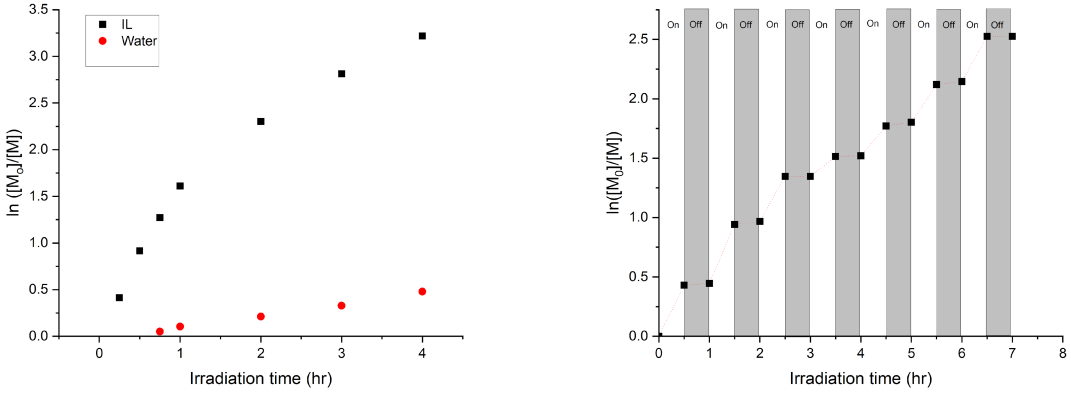

Figure 1: (a) Kinetics of photo-iniferter RAFT polymerization of dimethyl acrylamide in ionic liquids compared with the same in water (b) The temporal control of the photo-iniferter RAFT polymerization in ionic liquids.

Reversible addition-fragmentation chain transfer (RAFT) polymerization is one of the important reversible deactivation radical polymerization (RDRP) techniques known for its versality and ability to synthesize polymers with well-defined molecular weights and architectures. By using visible light, as an external stimulus, it is possible to selectively excite the spin-forbidden n -> π* electronic transition in the RAFT agents[1], which would undergo β-cleavage and generate radicals. Thus, the RAFT agents can be used as iniferter agents for polymerization under visible light[2]. Although this process is free of external catalysts and initiators, it is extremely slow. This study shows that the use of ionic liquids as reaction media would speed up the photo-iniferter RAFT process. We also demonstrate the robustness of the process in synthesizing linear polymers, block copolymers and stars using acrylamides and acrylates. The process is not only well controled but can also be temporally controlled and high chain end fidelity is obtained under 5 hrs of irradiation time.

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Lake Records from northern and eastern India and model runs to understand monsoon variability during the last millenium

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Abstract

Lakes are an excellent continental proxy that preserve sediments, pollen as well as other microfauna, and bears geochemical signatures to infer palaeoclimatic variations in the past. To understand monsoon variability during the last millennium, we have chosen two lakes, Anshupa Lake, Odisha, and Lahuradewa, Uttar Pradesh. Five sediment cores (max length: 1.4m) were obtained from Anshupa lake by a Gravity Corer and have been sub-sampled at every 5 mm interval. We plan to obtain longer cores (10 m) from these lakes in the coming year. These cores will be dated using the AMS ^{14}C dating technique. Multiproxy analyses such as particle size analysis, trace-element ratios (such as Mg/Ca, Rb/Sr, Al/Ti), C/N ratios, environmental magnetism, and biomarkers will help in developing energy models, understanding the lake environment, paleo-aridity and changes in rainfall and temperature. We propose to run a global climate model using lake proxies for the last 2000 years and compare these results with other existing global climate models to identify the suitable model(s) over this region. From rigorous comparisons between the output from numerical simulations and paleoclimatic data, we can investigate the past and study the drivers of climate variability and changes in the future. The records also will help to demonstrate the globally known climate events such as the Medieval Climate Anomaly (MCA), Little Ice Age (LIA), and Maunder Minimum. Our research is robust and has great socio-economic-academic value for the South Asian communities in particular and global community in general for their interest in climate variability.

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Keywords: Lake sediments, Paleoclimate, Climate modelling

Global and regional (Southern Ocean) timeseries analysis of Chl-a concentration and study of its correlation with physical processes

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Abstract
Marine phytoplanktons account for about 45 percent of global net primary productivity and play an important role in the global carbon cycle. The abudance and availability of phytoplanktons in the ocean depends primarily on the availability of light and nutrients (both micro and macro nutrients). Many environmental parameters such as sea surface temperature (SST), mixed layer depth (MLD), wind stress, currents, etc. also affect the population of phytoplanktons. These variables are, in fact, modulated by different physical and biological processes in the ocean. In this study, the roles of different physical processes affecting the supply and distribution of nutrients to phytoplanktons are studied, and also how they affect the chlorophyll-a (Chl-a) concentration, an index of phytoplankton concentrations. Merged satellite ocean color data from ESA's GlobColour project were investigated for the period of 23 years between 1997 and 2019 to analyze the timeseries of global and regional (SouthernOcean) Chl-a concentration. From the analysis, it was found that Chl-a concentration showed increasing trend of 0.015 mg/m3 globally and 0.062 mg/m3 over the Southern Ocean (SO) with p-value less than 0.01. It was also found that most of the increasing trends are shown spatially in the open ocean and decreasing trend in the coastal regions during the study period. The correlation of Chl-a with different environmental parameters such as SST, windstress, MLD,etc. are also been studied.

Keyword
Phytoplanktons, Southern Ocean, ocean color

Structure-function insight into the two-component NHEJ DNA repair system of *Mycobacterium tuberculosis*

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Abstract

Double stranded break (DSB) is considered to be the most detrimental form of DNA damage encountered by living systems across species. If not readily repaired, a single DSB is sufficient to arrest all cellular processes [1]. In nature, DSBs are induced by environmental factors (ionizing radiation and chemical agents) and endogenous byproducts (Reactive oxygen and nitrogen species). Thus, double-stranded break repair (DSBR) is critical for genomic stability and sustenance of any living system. Eukaryotic organisms employ a large number of factors to repair DSBs by Non-homologous end joining (NHEJ). A functionally similar repair apparatus composed of Ku and a multifunctional DNA ligase (Ligase D) have been identified in many prokaryotes. Bacterial NHEJ complex is a two-component system that, despite its relative simplicity, possesses all of the break-recognition, end-processing, and ligation activities required to facilitate the complex task of DSBR [2]. The significance of NHEJ repair for intracellular pathogens is invaluable, especially in non-replicating or dormant phases of the lifecycle. Like most other prokaryotes, *Mycobacterium tuberculosis* employs its two-component machinery for DSBR with probable aid from a homologue of VCP/p97 (Proteasome involved in the regulation of eukaryotic NHEJ pathway) [3]. This research aims to unravel the molecular mechanism of the NHEJ repair pathway of *M.tuberculosis* (H37Rv) by structural and functional analysis of its two-component system and its involvement with Mycobacterial proteasomal ATPase (VCP/p97 homologue).

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Keywords
Mycobacterium tuberculosis; Non-Homologous End Joining; Mycobacterial proteasomal ATPase

Investigation of chemical and physical effects from acoustic bubble(s) in partially-degassed liquid

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Abstract
Ultrasound (acoustic waves with frequency > 20 kHz) plays an important role in biomedical and engineering applications e.g. histotripsy/lithotripsy, food and dairy industry, nanoparticle generation etc. It helps generate several bubbles in bulk liquid from pre-existing gas nuclei, that oscillate and collapse either gently or violently in the presence of ultrasound. This process helps unlock several physical (jet, shockwave , streaming) and chemical (free radical generation) effects, which have been extensively studied. However, at low gas concentrations, when the amount of dissolved gas nuclei get substantially reduced, certain hypothesis point out that the nature of bubble formation and collapse would vary significantly. This would have an indirect influence on the nature of the resulting chemical and physical effects. But difficulty of controlled experiments have led lack of knowledge in this sector. Experiments using small volumes of partially degassed liquid (created by reducing overhead gas pressure) is generally used that is susceptible to gas intrusion from outside, sensitive to overheating and offer very small measurement times for chemical effects. Physical effects on the other hand require isolating single acoustic bubble for sufficient time under suitable optical conditions for data acquisition.
In the current work, the above problems and feasible solutions have been discussed to explore acoustic cavitation under stringent gas conditions. The nature of physical (particular streaming) and chemical (sonochemistry) effects are also briefed at the same condition.

Keywords: streaming, sonochemistry , air-water interface

Self assembly Simulation and Modelling of organic OPV nano-materials

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Abstract
Our work contributes in predicting effects of OPV materials in solar cell active layer through MD simulations. Through general coarse grained simulations, the rate of change of component solubility, demixing tendency, and the difference in interaction energies, were studied for nano-composite self-assemblies. Routes to form uniform, core-shell, Janus, eccentric morphologies were established. Using atomistic simulations it was established that increasing P3HT chain length the stability of the nanocomposite (P3HT:PCBM/ICBA) decreases, whereas increasing PDI stability increases. Also answered why BTR and BQR of the entire BXR series (benzodithiophene- X-thiophene-rhodamine) exhibit liquid-crystalline phase and highest PCE in solar cell usage.

Keyword (*max 3*)
self assembly, molecular dynamic simulations, composite opv nano-particles

Contact Angle Hysteresis on Surfaces with Random Topology

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Abstract
Surface wetting is ubiquitous in nature and has many applications including the mining and separation of metal ores, enhanced oil recovery and the production of self-cleaning surfaces etc. Contact angle measurement serves as the basis for quantifying surface wettability. However, the available models [1,2] are not capable of predicting the contact angle on real surfaces. The contact angle not only depends on the physical and chemical properties of the surface but also upon the history of the droplet. The difference between the contact angles during volume increasing (advancing) and decreasing (receding) modes is known as contact angle hysteresis (CAH). Even on a chemically homogeneous surface, the presence of surface roughness alone can generate hysteresis. The situation becomes more complex on real surfaces, which have a random roughness. In this paper, we show the hysteresis measured experimentally on surfaces with cylindrical pillars (height = diameter =10 μm) with a known average area fraction. The results are presented for wetting of micropatterned silicon wafers coated with a monolayer of octadecane thiol with water. We observed multiple contact angles at which the interface de-pins and advances/ recede which is counterintuitive. We also present a numerical model (developed using the open-source software Surface Evolver) based on the dissipation of energy [3] during the contact line jump. We observed a good agreement between the experimental data and the numerical model, which can predict the contact angle hysteresis on real surfaces from the knowledge of the surface topography.

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Keyword
Contact Angle Hysteresis, Random Surfaces, Surface Evolver

Petrogenesis of coeval lamproites and kimberlites from the Wajrakarur field, Southern India: new insights from olivine compositions

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Abstract

Olivine is one of the most abundant phases in kimberlites and cratonic lamproites, where it occurs as mantle-derived xenocrysts and magmatic phenocrysts or rims overgrowing xenocrystic cores, indicating its prevalence throughout most of the crystallization sequence of these magmas. Thus, olivine can provide valuable insights into kimberlite and lamproite petrogenesis. Here, we present a detailed study of olivine compositional zoning in two lamproites (P2 and P12) of the Mesoproterozoic Wajrakarur kimberlite-lamproite field in southern India and use these data to propose a genetic link between lamproites and kimberlites in the region. To evaluate potential petrogenetic links between coeval lamproites and kimberlites from Wajrakarur, the composition of olivine xenocrysts (i.e., macrocryst cores) was compared with that of early crystallised olivine in P2, P12 and previously studied kimberlites and lamproites. The average Mg# of olivine macrocryst cores is directly correlated with the average Mg# of magmatic olivine in lamproites and kimberlites from Wajrakarur. Coupled with their indistinguishable Sr-Nd-Hf isotope compositions, these data suggest derivation of the Wajrakarur lamproites and kimberlites from a common source, The more Fe-rich composition of liquidus olivine in the Wajrakarur lamproites compared to coeval kimberlites suggests a higher degree of assimilation of metasomatised Fe-richer lithospheric mantle by the lamproites and provides a plausible explanation for the different petrological features of the Wajrakarur lamproites and kimberlites Our results suggest that cratonic lamproites can have a remarkably similar petrogenetic history to kimberlites.

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Keyword

Lamproite; Olivine; Zonation

Traffic state estimation using crowd-sourced data without road sensors

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Abstract

Traffic state estimation in any city is necessary for improving socio-economic conditions, and reducing environmental pollution, excess energy consumption, significant public health issues and interrupted traffic movement of that city. Traffic state estimation (TSE) infers estimation of various traffic state variables e.g., flow (veh/h), density (veh/km), travel time, and velocity (km/h) [3]. The aforementioned traffic state variables can be directly derived from the followings: (i) origins
and destinations of vehicles (OD flow)[2], (ii) arterial travel time (link travel time), (iii) arterial traffic counts (link counts), and (iv) parking locations and occupancy information [2, 1]. Thus, estimation of traffic state variables (or traffic state) can be done with the knowledge of OD flow, travel time, link counts, and parking information of a road-network.

Previous research on estimating OD flow, link count, and parking information has been done using expensive sensor-based transportation data, subject to be available depending on city's transport infrastructure [3, 1]. However, many developing cities lack sensor-based transport infrastructure for traffic state estimation directly. Eventually, lack of transport state information is becoming a challenge to these developing cities' growing economic opportunities that can lead to an economic dead end. Hence, the motivation of this research is find an alternative solution that will reduce the sensor-based infrastructure dependencies such that unavailability of these expensive data will not
restrict to gain sufficient knowledge about the city traffic state. This research can be further used for economic and ecological loss control, as well as traffic operations and planning in developing cities.

Keywords

Traffic state estimation, crowd-sourced solution, trajectory data.

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Resource Allocation Policies for 5G/6G Applications in Access Networks with Optimization and AI

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Abstract

With the advent of 5/6G, new applications such as AR/VR, remote surgery, internet of vehicles must be supported by the network. These applications require satisfying stringent quality of experience (QoE) requirements. At the access segment of the network, the traffic is usually bursty compared to that of core networks which makes conventional allocation policies like Diffserv to be incapable of handling such QoE requirements. Moreover, most of the available literature caters to QoE constraints in the average sense instead of going for a robust or design.

In our work, we show how strict QoE requirements can be modeled and satisfied in popular access networks such as Passive Optical Networks (PON) and Radio Access Networks (RAN). In PON, we show how Model Predictive Control (MPC) technique can be used for deciding dynamic bandwidth allocation policies that satisfy QoE requirements. In the backhaul, we focus on end-to-end QoE satisfaction with help of modern networking and computing orchestrators like software defined networks (SDN) and Kubernetes. We show how QoE requirements can be modeled with help of AI and subsequently use robust optimization for allocating resources (often termed as slicing [1] in context of SDN).

Keyword
Access Networks, uRLLC, E2E QoE, SDN, Kubernetes

[1] https://www.ericsson.com/en/network-slicing

Integrated Urban Water Balance Model for Developing Countries

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Abstract

Urban water supply systems in developing countries like India face unique water-related problems or challenges due to changing socio-economic dynamics, pollution of water sources, depletion of limited freshwater availability and climatic change. The challenges contribute significantly to intermittency in piped-water supply in India, where piped-water service typically delivers less than 24 hours a day or a particular number of days per week in some cases. It is important to analyze water balance in developing countries so that necessary modifications can be made to make sufficient water available, thus increasing the reliability of water services supplied.

Integrated Urban Water Management (IUWM) is one of the principles applicable to integrated water management in urban areas, and it relies on diversifying water sources, integrating all the parts of the water cycle to produce fit-for-purpose water. Such principles utilize various sustainability approaches based on water conservation, reuse and recycling involving multiple stakeholders, water experts, planners and communities in the decision-making process, and presents potential solutions to achieve supply reliability in developing countries.

Several water simulation platforms have been developed to model urban water supply integrating IUWM principles and have been used largely in developed countries. We developed an IUWM incorporated model using eWater Source Version 5.4.0.11797 to analyze improvement in water supply reliability, with Bangalore, India, as a case study. Five different supply configurations to incorporate IUWM principles were analyzed and compared to identify the most efficient way to incorporate non-conventional water sources (e.g., harvested stormwater, rooftop rainwater, and recycled wastewater). The supply reliability of the current water supply and improved water supply was then compared.As compared to the current water supply configuration, all the IUWM incorporated urban water supply configurations produced much higher water supply reliability results.

Keyword
Integrated Urban Water Management (IUWM), urban water supply systems, developing countries

Increasing efficiency of high-lift turbine blades with roughness and riblets

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Abstract
Low-pressure turbines in aircraft engines employ high-lift blade designs that are susceptible to undesirable flow separation. Past research have shown the favourable effects of the free-stream turbulence, unsteady wakes from the upstream blades and surface roughness due to in-service degradation towards mitigating the separation bubble related losses over the blade suction surface. However, some of the benefits are offset by an increase in the loss associated with a larger turbulent wetted area. In this work, we will discuss the results of a transitioning boundary layer with and without streamwise varying pressure gradients (SPGs). We explore the loss reduction strategies by employing roughness elements to suppress the separation bubble and riblets to reduce the viscous turbulent drag. The Boundary Data Immersion Method (BDIM) is employed to represent the roughness and riblets while a digital filtering approach is used to impose free-stream turbulence (FST) at the inlet. The performance of different riblet shapes in conjunction with the roughness elements will be demonstrated through boundary layer integral parameters, skin friction coefficient etc for several test cases. Time, span and phase averaged turbulent statistics will be presented in discerning the influence of riblets close to the wall.

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Keywords
LPT, roughness, riblets

Structural and functional changes at the knee after anterior cruciate ligament reconstruction

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Abstract

The (Human) knee is a complex system consisting of three bones and two joints: the femur and tibia articulate at the tibiofemoral joint; and the femur and patella, at the patellofemoral joint. The three bones with other connective tissue like the tendons, ligaments and, cartilage work in sync with the musculoskeletal system and the neural system to achieve stability and mobility of the joint while performing various routine and complex activities. The structure and function of the knee joint are interdependent and change in one affects the other. Damage to the knee ligaments and menisci can lead to abnormal bone motion that alters the strains imposed on cartilage and increases the risk of osteoarthritis (joint disease). The Anterior-cruciate-ligament (ACL) at the knee is one of the most researched ligaments due to its frequent injury. ACL reconstruction is performed to restore knee stability and function and preserve joint health. However, clinical studies with long-term follow-up indicate that up to 90% of individuals undergoing ACL reconstruction have radiographic evidence of osteoarthritis in both the tibiofemoral and patellofemoral joints within 10 years. The aim of this study was to understand the structural and functional changes at the knee joint by analyzing the change in ligament attachment sites, three-dimensional moments at the knee joints, and the patellar tendon moment arm and comparing these between the ACL reconstructed knee and the contralateral knee. By doing so we might be able to design better surgical procedures, rehabilitative methods post, and pre-surgery to prevent further degradation at the joint.

Keyword
Patellar tendon moment arm, Anterior cruciate ligament reconstruction, Three-dimensional moments

Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study

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Abstract

Quantum chemistry and statistical reaction rate theory calculations have been performed to investigate the products and kinetics of indenyl radical decomposition. Three competitive product sets are identified, including formation of the cyclopentadienyl radical (*c*-C_5H_5) and diacetylene (C_4H_2), which has not been included in prior theoretical kinetics investigations. Rate coefficients for indenyl decomposition are determined from master equation simulations at 1800 - 2400 K and 0.01 - 100 atm, and temperature- and pressure-dependent rate coefficient expressions are incorporated into a detailed chemical kinetic model for indene pyrolysis. Indenyl is found to predominantly decompose to *o*-benzyne (C_6H_4) + propargyl (C_3H_3), with lesser amounts of fulvenallenyl (C_7H_5) + C_2H_2 and *c*-C_5H_5 + C_4H_2.

Keywords

Reaction kinetics; Indenyl; PAH

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