

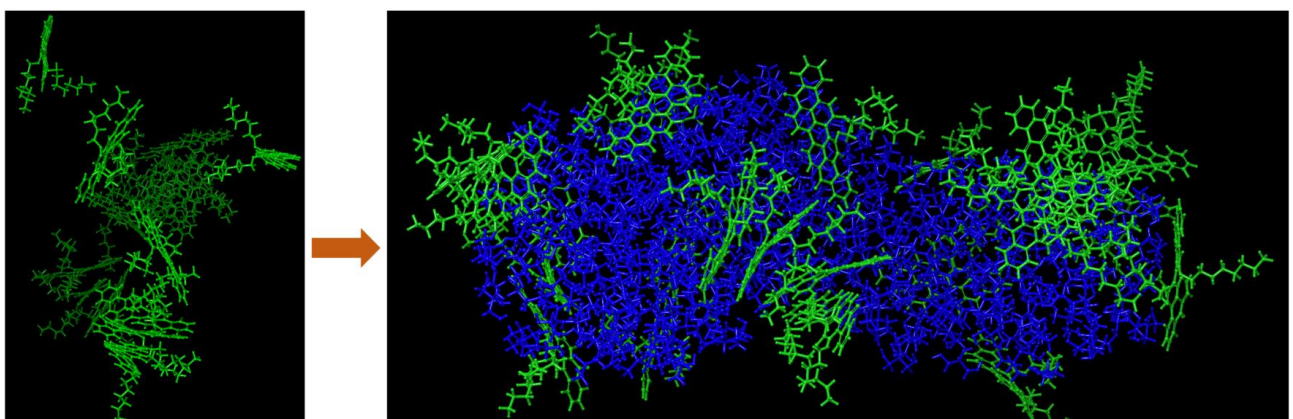


TEMPUS

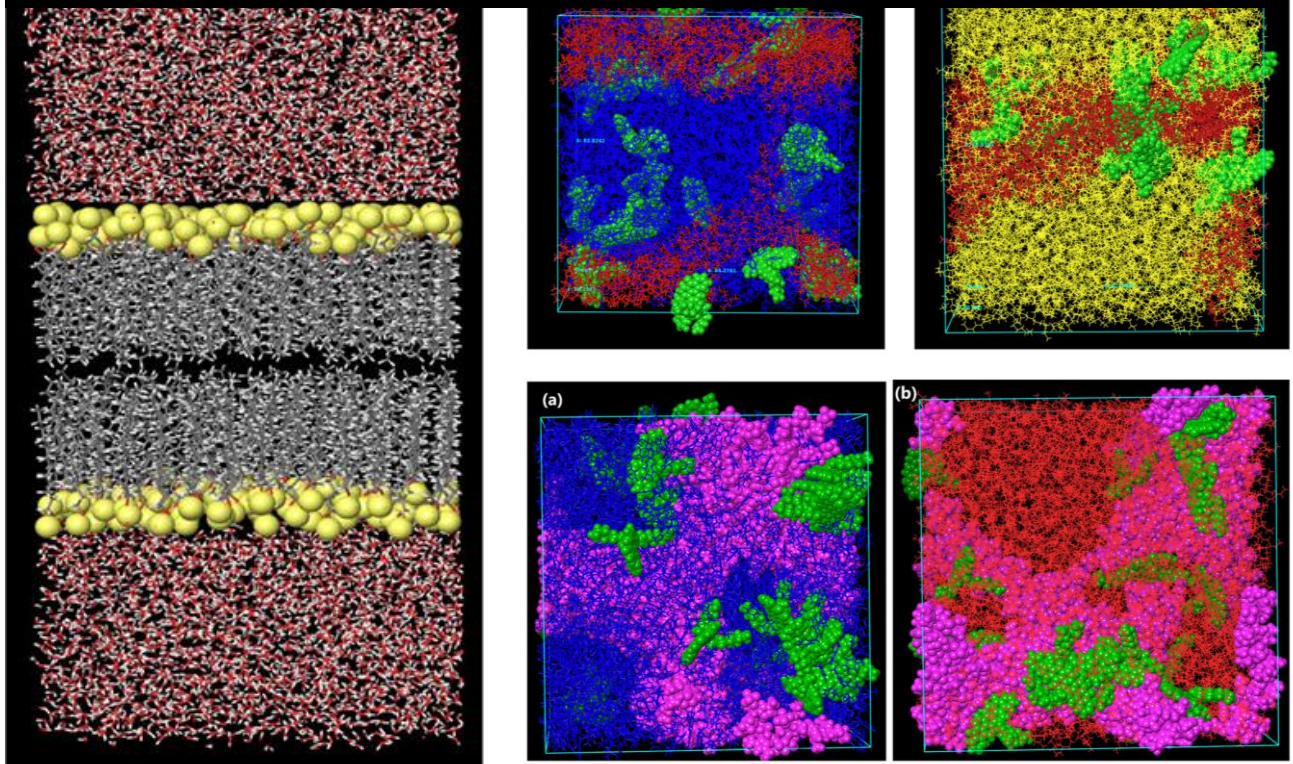
Newsletter Department of Chemical Engineering

VOLUME - 4

JULY 2024



Molecular Simulations in Action



Best Research Department
2024 at MIT, Manipal

Felicitations of Alumnus
Mr. Shyam Kamath, MD, MRPL, Mangalore

Farewell to
Dr. K. Balakrishna Prabhu

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From the HOD's Desk

Dear Readers,

I am glad to present the July 2024 issue of our department's newsletter. In this issue, we showcase the latest updates and accomplishments and highlight the talent and dedication within our department. Research updates, faculty and student achievements, and exciting event highlights are on these pages. I encourage you to read, engage, and share your thoughts.

The past few months have been filled with events highlighting our commitment to academic excellence, research innovation, and strong alumni connections.

Our department had initiated an agreement with CDAC, Bengaluru, and in collaboration, organized a highly successful two-day workshop on "HPC & Parallel Programming" in January 2024. This event provided our students and faculty hands-on training in high-performance computing, a crucial skill in modern chemical engineering research and industry applications. Further, I am proud to announce that our department was honoured with the "Award for Excellent Research Performance" in the Engineering category at the MIT Research Day function held on April 17th, 2024. This prestigious award is a recognition of the collective efforts of our faculty and students, whose research continues to contribute significantly to the field of chemical engineering.

We had the privilege of hosting Dr. Mohammad Khalid, Professor and Head of the Sunway Centre for Electrochemical and Sustainable Technology, Malaysia, and Adjunct Faculty in our department during his two-week academic and research visit.

We recently organized a farewell for Dr. Balakrishna Prabhu K, a valued colleague who has made significant contributions to our department.

In a special ceremony, we felicitated our distinguished alumnus, Mr. Shyam Kamath, Managing Director of MRPL, Mangaluru. Mr. Kamath has been a pillar of support for our department, and his professional achievements inspire our students.

These events and achievements highlight the vibrant and dynamic environment within our department. I am confident that, with the continued support of our faculty, students, and alumni, we will continue to achieve new heights in teaching, research, and community engagement.

Best regards,

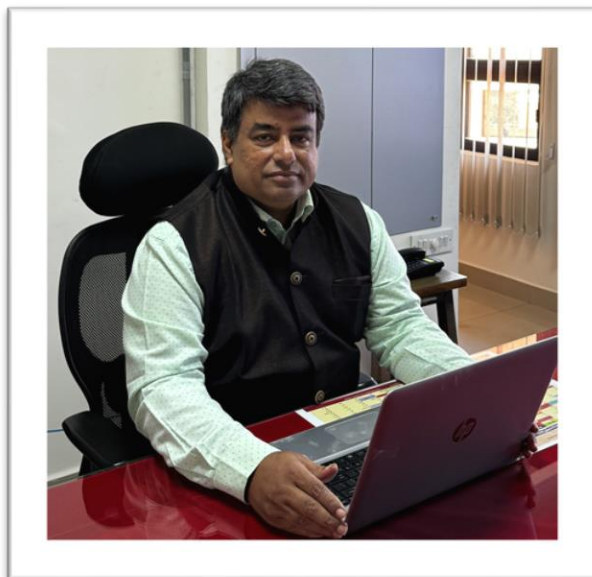
Dr. M. Srinivas Kini

Professor & Head,

Department of Chemical Engineering

Manipal Institute of Technology, MAHE, Manipal-576104.

Email: srinivas.kini@manipal.edu



Department Events

MAHE-CDAC Agreement Exchange Ceremony



January 2, 2024 marked a pivotal moment in the annals of academic-industrial collaboration as **Manipal Academy of Higher Education (MAHE)** and the **Centre for Development of Advanced Computing (CDAC), Bengaluru** forged a strategic alliance. The collaboration between **MAHE** and **CDAC**, spearheaded by **Dr. Srikanth Divi** and overseen by **Commander (Dr.) Anil Rana**, is poised to elevate MAHE's research capabilities to unprecedented heights.





The signing of the **MAHE-CDAC** Service Level Agreement (SLA) at the EDU Building in Manipal was a momentous occasion of intellectual exchange that brought together esteemed dignitaries from both institutions. The event was graced by the presence of **Lt. Gen. (Dr.) M. D. Venkatesh**, Vice Chancellor of MAHE; **Dr. Narayana Sabhahit**, Pro Vice Chancellor (Technology & Science); **Dr. P. Giridhar Kini**, Registrar; **Commander (Dr.) Anil Rana**, Director of MIT; **Dr. Srikanth Divi** (Chemical), **Mr. Satish Kamath**, Deputy IT Director and **Dr. Neha** (CSE). From CDAC, **Executive Director Dr. S. D. Sudarsan**, **Associate Director Dr. Mohammed Misbahuddin**, **Joint Director Mr. P. Soundararajan**, and **Principal Technical Officers Mr. B. Arunachalam** and **Mr. Raghu H. V.** were in attendance.



A Quantum Leap in Research and Innovation

The strategic partnership will empower MAHE's research scholars, students, and faculty with access to CDAC's state-of-the-art supercomputing facilities, including the formidable Param Utkarsh. This cutting-edge infrastructure will serve as a catalyst for groundbreaking research across a diverse spectrum of domains, from parallel programming and quantum computing to molecular simulations and artificial intelligence.

A Catalyst for Academic Excellence

By leveraging CDAC's expertise and resources, MAHE aims to foster a culture of innovation, drive research excellence, and contribute significantly to the advancement of knowledge in these critical areas. This partnership represents a quantum leap forward in MAHE's journey to become a global higher education and research leader.

Focus on Emerging Technologies: The emphasis on quantum computing, IoT, and cybersecurity indicates CDAC's alignment with emerging technological trends.

Comprehensive Training: The range of programs, from BTech to postgraduate diplomas and certifications, offers a comprehensive approach to training in advanced computing. CDAC offers internships for UG and PG students on their campus.

Industry Relevance: The collaboration with IEEE and the focus on practical skills like DNS receiver strongly emphasise industry relevance. CDAC also offers exclusive training and certification programs in collaboration with IEEE.

Access to High-Performance Computing: The inclusion of supercomputer access provides students and researchers with the opportunity to work on large-scale computational projects.

Opportunities for education and training: CDAC's training programs offer individuals the chance to acquire valuable skills and knowledge in advanced computing.

Collaboration and networking: CDAC's collaborative environment provides opportunities to connect with experts and researchers in the field.

Support for research and development: CDAC's consulting services and research projects can support organizations in their own research and development efforts.

KEY AREAS OF FOCUS

- PARALLEL PROGRAMMING
- QUANTUM COMPUTING
- MOLECULAR SIMULATIONS
- INTERNET OF THINGS (IOT)
- ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING
- CYBERSECURITY
- COMPUTATIONAL FLUID DYNAMICS (CFD)
- GPU PROGRAMMING
- SEMANTIC MINING
- BIG DATA
- INTELLECTUAL PROPERTY RIGHTS (IPR)
- TECHNOLOGY

HPC & Parallel Programming Workshop



The Department of Chemical Engineering had organized a two-day workshop on "HPC & Parallel Programming" from 4th January 2024 to 05th January 2024 at Manipal Institute of Technology (MIT), Manipal. The workshop aimed to provide hands-on training sessions on various topics related to high-performance computing (HPC) and parallel programming, such as using the CDAC supercomputer facility, OpenMP/MPI, AI software stack, quantum computing, and molecular simulations. Over 120+ registrations were received for the event, and the workshop was attended by all faculty members, research scholars, and students of MIT and other MAHE institutions.

The workshop was inaugurated by Cdr. (Dr.) Anil Rana, the Director of MIT, inspired the participants and highlighted the importance of HPC and parallel programming for academia, advancing scientific research and innovation. He also thanked the CDAC team for their collaboration and support in conducting the workshop. The CDAC team consisted of Mr. Soundararajan, Mr. Arunachalam, and Mr. Raghu, the resource persons for the training sessions.

The first day of the workshop focused on the basics of HPC and parallel programming, involving the architecture and features of the CDAC supercomputer facility, the concepts and principles of parallel programming, and the introduction to OpenMP and MPI. The participants gained operational skills of the CDAC supercomputer facility, learned program writing using OpenMP and MPI, and cultivated knowledge on measuring and enhancing the performance of parallel programs. The sessions were interactive and involved hands-on exercises and examples.

The second day of the workshop covered further advanced topics, such as the AI software stack and molecular dynamics simulations. The participants learned about the various tools and frameworks for developing HPC applications using the CDAC supercomputer facility. Finally, they explored the applications of molecular dynamics simulations in materials science and other fields. They also learned to use NAMD, GROMACS, and LAMMPS to conduct molecular dynamics simulations utilizing the CDAC supercomputer facility. By using these software packages on CDAC's supercomputer facility, researchers can:

Simulate the dynamics of molecules and materials: This helps to understand the behavior of these systems at the atomic and molecular level.

Study the properties of materials: Simulations can be used to investigate properties such as mechanical strength, conductivity, and reactivity.

Design new materials: Simulations can aid in the design of new materials with specific properties.

Investigate biological processes: Simulations can be used to study biological processes, such as protein folding and enzyme catalysis.

The workshop concluded with a feedback session and a valedictory ceremony. The participants expressed their satisfaction and appreciation for the workshop and thanked the organizers and resource persons for their efforts.

Visit of Dr. Khalid M to the Department

Dr. Mohammad Khalid, Professor and Head Sunway Centre for Electrochemical and Sustainable Technology, Malaysia, and Adjunct Faculty in the Department of Chemical Engineering at MIT, was on two-week academic and research visit from 22nd January to 05th February. During his stay, Dr. Khalid engaged with our faculty and shared his expertise with students from the 4th, 6th, and 8th semesters of the B.Tech program along with the students from 2nd Semester of the M.Tech program and PhD scholars. His interactions were insightful and inspiring, fostering a collaborative learning environment and providing valuable guidance to both students and faculty members.



Farewell of M.Tech II Semester students

The farewell for the M.Tech students was organized in April, 2024 at Hampi Hall. It was a fun-filled afternoon, brimming with joy and camaraderie. Both students and faculty participated enthusiastically, creating a lively and memorable event. The celebration featured engaging games, heartfelt speeches, and entertaining performances, fostering a sense of unity and nostalgia. It was a perfect blend of laughter, reflection, and goodbyes, making it a cherished day for everyone involved.



Best Research Department Award

At the MIT Research Day function on 17th April 2024, held at the Library Auditorium, our Department was honored with the “Award for Excellent Research Performance” in the Engineering category. This prestigious accolade recognizes our outstanding contributions and dedication to advancing engineering research. The event gathered esteemed academics and researchers and highlighted the most innovative and impactful work across various disciplines. Receiving this award is a testament to our hard work and commitment to excellence, inspiring us to continue pushing the boundaries of engineering knowledge and innovation. Dr. Raja S. was honoured with the Best Researcher Award for 2023 at the MIT Research Day function. Remarkably, he also received this prestigious award in 2022.



Farewell to Dr. K. Balakrishna Prabhu

On the 6th of May 2024 at 11:30 AM, a heartfelt farewell ceremony was held in honour of Dr. Balakrishna Prabhu K (Former Professor & HoD), marking the end of his illustrious tenure as a professor at our institution. The event was graced by Director Dr. Anil Rana, Joint Director Dr. Somashekhar Bhat and HoD Dr. M Srinivas Kini, along with esteemed faculty members, staff, and students from the department. Faculty members and staff took the stage to share their memories and express gratitude, followed by felicitation to Dr. Balakrishna Prabhu K. We extend our deepest gratitude to Dr. Prabhu for his 35 years of dedicated service and wish him a fulfilling and joyous retirement. Thank you, Dr. Prabhu, for your exceptional contributions to the Chemical Engineering Dept. and MIT, and for inspiring us all.



Felicitation of Mr Shyam Kamath, MD, MRPL, Mangalore

On June 3rd, 2024, Mr. Shyamprasad Kamath, MD of MRPL, Mangalore, was felicitated at his office by Dr. Harish Kumar, Professor & Director of Corporate Relations at MAHE, Dr. Kanthi, Associate Director of Alumni Affairs, and Dr. M. Srinivas Kini, Head of the Chemical Engineering Department. This event recognized Mr. Kamath's outstanding industry contributions and ongoing support and collaboration with MAHE. The occasion was marked by heartfelt appreciation and discussions on future initiatives to strengthen industry-academic partnerships.



IICHE STUDENT CHAPTER MANIPAL – Event Details

Board Transfer

Board transfer of the Indian Institute of Chemical Engineers, student chapter Manipal was conducted on 31 Oct 2023 commencing, the tenure of selected candidates.



Event 1: ChemStrikers Challenge - IICHE Cup Edition

- **Title of the event:** ChemStrikers Challenge - IICHE Cup Edition
- **Date and time:** 17-01-24 at 5:00 PM
- **Venue:** MIT Football Ground
- **Brief synopsis of the event:**

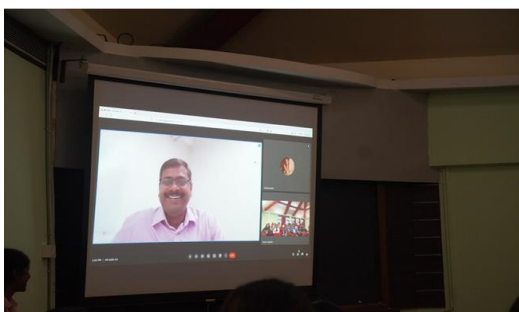


IICHE held a football team bonding event on January 17th, filled with enthusiasm, joy, and cooperation. The perfect execution of the IICHE team has been a major factor in bringing this gathering to such great success. Four teams were in the tournament, creating a sense of comradeship among the players. All the refreshments were freely distributed to ensure everyone felt refreshed throughout the day.

Event 2: Crafting a Mind-Blowing Resume for Engineering Students

- **Title of the event:** Crafting a Mind-Blowing Resume for Engineering Students
- **Date and time:** 30-01-24 at 5 PM | **Venue:** Hampi Hall, AB 2
- **Brief synopsis of the event:**

The goal of the 30th of January IICHE Manipal Student Chapter Resume Building Workshop was to provide participants with the fundamental know-how and abilities needed to write a strong CV. Prominent speakers at the workshop included Dr. Anoop Kishore V, assistant professor at the Department of Chemical Engineering, MIT, and Mr. George Cardoz, Head of HR at Forbes Marshall. They shared their knowledge on effective resume building and provided insightful advice on how to construct resumes that stand out in a crowded job market, giving listeners useful advice on how to customize resumes for various industries, with a focus on action verbs, emphasizing major accomplishments, and tailoring resumes to fit employment needs.



Established “Augmented Intelligence and Molecular Simulations” (AIMS) Lab



The newly established AIMS Lab at the Department of Chemical Engineering is dedicated to pioneering research in augmented intelligence and molecular simulations. This interdisciplinary lab aims to revolutionize energy storage, drug delivery, nutraceuticals, and machine learning by leveraging advanced AI techniques to enhance molecular simulations. Through groundbreaking research, the AIMS Lab seeks to address critical challenges and develop innovative solutions for a sustainable future.

The AIMS Lab will utilise computational tools to perform molecular simulations and extract meaningful insights from complex data. **Discover materials** with enhanced properties for energy storage and drug delivery. **Develop innovative nutraceuticals** with improved bioavailability and efficacy. **Apply machine learning models** to predict molecular properties.

The AIMS Lab is committed to fostering collaborations with industry partners and other research institutions to translate its research findings into real-world applications.



Faculty Achievements

Grants Awarded to Faculties



Dr. Anoop Kishore V. Assistant Professor, MIT Manipal in collaboration with **Prof. Tamal Banerjee**, Department of Chemical Engineering, IIT Guwahati, received a research grant of **Rs 15 lakhs** on a project titled "**Reaction Kinetics Pathways of Liquid Organic Hydrogen Carriers for Effective Hydrogen Storage Using Ab Initio Calculations.**" for a period of 2 years in January 2024 from SERB under Teachers Associateship for Research Excellence (TARE) Scheme.



Dr. Jitendra Carpenter, Assistant Professor, as PI and **Dr. Anoop Kishore V.** as Co-PI received a research grant of **Rs 40 lakhs** for a period of 2 years in February 2024 from VGST, Govt of Karnataka under GRE Scheme for the establishment of Centre of Excellence in a the project titled "**Design and Development of low energy hydrodynamic cavitation-based homogenizer for the synthesis of food and pharmaceutical grade oil-in-water nanoemulsions: Experimental & Molecular Simulations Insights**"



Dr. Raja S. Professor, MIT Manipal received a grant of **Rs 03 lakhs** in February 2024 from VGST, Govt of Karnataka under FDP Scheme to conduct an FDP on "**Advances and Recent Trends in Environmental and Energy Applications of Nanomaterials**".



Dr. Anoop Kishore V., and Dr. Srikanth Divi in collaboration with Dr. Poulumi Dey TU Delft, Netherlands (QS World University Rankings 2025 # 49), published an article "Effectiveness of inhibitors to prevent asphaltene aggregation: Insights from atomistic and molecular simulations", J. Chem. Phys. 160, 090901 (2024) <https://doi.org/10.1063/5.0190779>. that was selected for Cover Page in Journal of Chemical Physics, AIP.

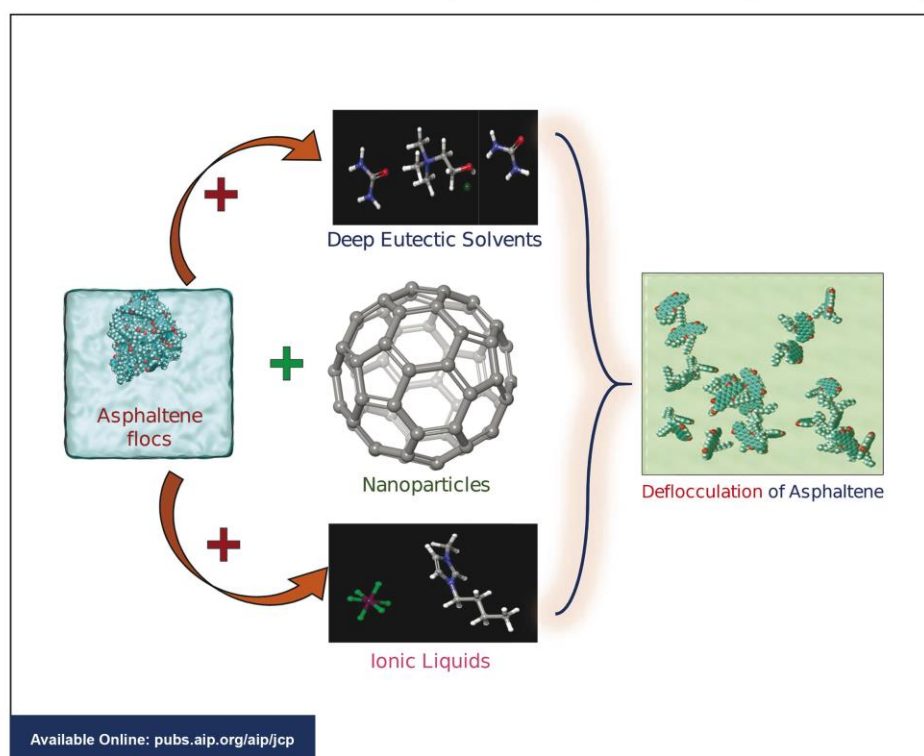
The Journal of Chemical Physics



Vol. 160, Iss. 9, 7 Mar. 2024

Effectiveness of inhibitors to prevent asphaltene aggregation: Insights from atomistic and molecular simulations

Anoop Kishore Vatti, Srikanth Divi, and Poulumi Dey



Student Achievements

Mohiet Iqbal (Reg. No. 210903028), a 3rd-year Chemical Engineering student, participated in the prestigious Yukti Innovation Challenge 2023. He collaborated with Abhay Singh Solanki from the Department of Electrical and Electronic Engineering. Their submission focused on sustainable manufacturing, addressing its crucial role in mitigating the adverse impacts of the fashion industry on our environment.

Out of over 10,000 teams nationwide, we are delighted to announce that their project has been recognized among the top 135 projects, earning a significant grant of 4 lakh INR which underscores the merit and potential of their endeavour.



Akansha Mohanty and Siddhika Ajmera (B.Tech. 5th Sem students) presented a review article on **“Thermo-Catalytic pyrolysis of sugarcane bagasse: A Py-GC-MS and XRF prospective”** in an International conference on Frontiers in Analytical and Applied Pyrolysis for Energy and Environment (FAAPEE)- 2024 at IIT Madras during 26 – 27 February 2024. They both worked under the guidance of Dr. Ranjeet Kumar Mishra, Associate Professor, MIT Manipal.



Anwesa Sarmah (B.Tech. 5th Sem) also presented a review article on **“Co- Pyrolysis of biomass and waste plastics to produce sustainable fuel and value added chemicals: A review”** under the guidance of Dr. Ranjeet Kumar Mishra, Associate Professor, MIT Manipal.

Fun Zone

WORD SEARCH PUZZLE! - Rishith Khanna

Words can be found in any direction (including diagonals) and can overlap each other. Use the word bank below.

T H E R M O C O U P L E O V O M C Q J F
E E Q H H R A M E H Z R E S N E D N O C
E R V S M O D E L L I N G J B Q V W B R
N U E R R C A I I F D B H K G B Z W P D
O M V K X S T A G O N U I E C C D T U K
N S U Q N L R E L I O B V G M T X T P O
Z H Y C H Z A S U P L E P D U P O D W M
I F T M Y Y Y N R Y T L W K P N W I R Z
F Y F Y M F S J E D V U B M T O H S K V
I F J O G R B G F Z S J Y F E K W T Q A
T F Q C H F J E I E Q J L K C H Y I Q N
X T H Z Z R G R N Y Y R R D Y Z O L R R
S E F L G G W C E Z C T J C N G P L P H
J K L O T C G O R B S U L V J I U A F G
T E T Z Q K V L Y C B V K P C D E T W P
P X A S P E N G L T S N O M L D I I T B
Y Z G U H I Y Z F L K U R K G O P O R M
Q M M B B S B M Y Z V S X U R V X N F A
F K X N P I N D D V D O J U K U X I T H
P Q W K F G H G U I U O N K S R Y T K H

1. Which process involves the separation of components in a liquid mixture through boiling and condensation? (Distillation)
2. Which type of reactor is designed to operate continuously, maintaining a uniform composition and temperature throughout? (CSTR)
3. What are the horizontal components inside a distillation column that provide surface area for vapor-liquid contact? (Trays)
4. Which facility processes crude oil into useful products like gasoline, diesel, and petrochemicals? (Refinery)
5. In distillation, what type of packing is often used to increase the surface area for vapor-liquid contact? (Mesh)
6. Which device measures temperature by using the voltage generated between two different metals? (Thermocouple)
7. Which piece of equipment is used to heat water and produce steam in various industrial processes? (Boiler)
8. What is the name of the popular process simulation software used in chemical engineering for design and optimization? (Aspen)
9. What term refers to the process of creating mathematical models to simulate real-world chemical processes? (Modelling)
10. In a distillation process, what piece of equipment is used to cool and condense vapor back into liquid? (Condenser)

Alumni Reminiscences

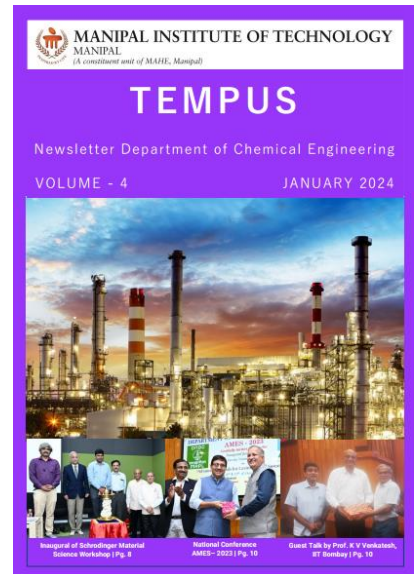
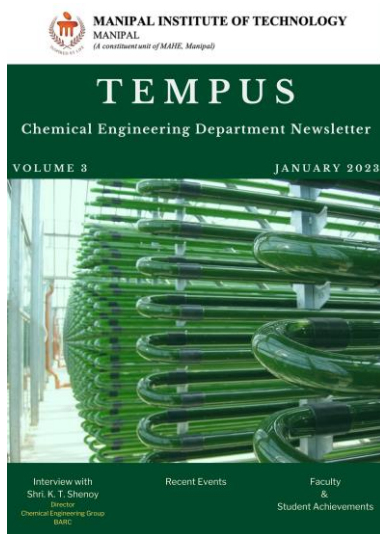
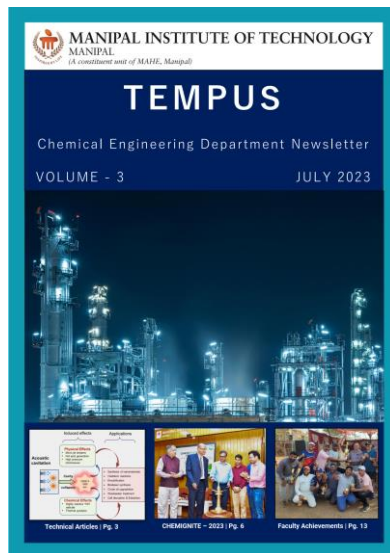
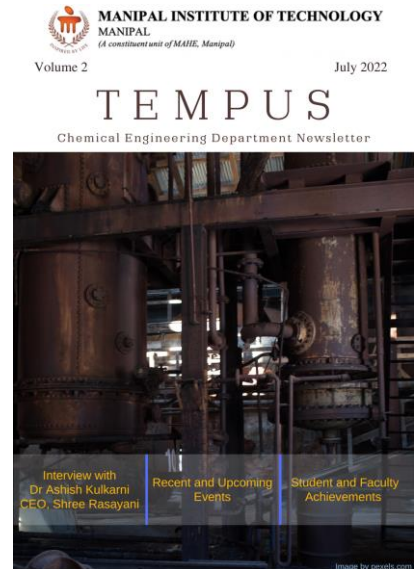
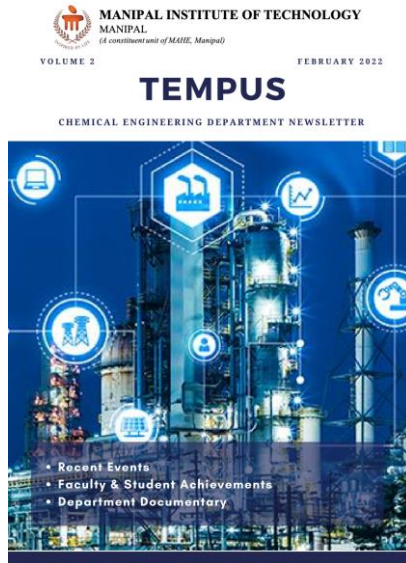
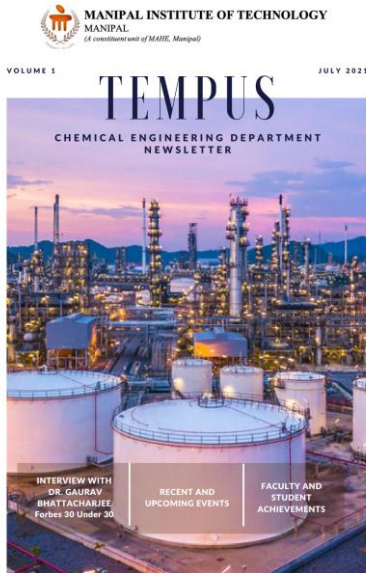
Here comes a fantastic opportunity for our MIT alumni. Pen down your best memories, thoughts, lessons, and experiences you have had on our campus in your college days and get them published in our next Tempus issue! Hoping to read the mind-boggling stories and epic pictures



<https://forms.office.com/r/rS8rY7SWf3>

TEMPUS Archives

Take a deep dive into our previous edition [here!](#)



Editorial Board



Dr Muddu Madakyaru



Dr Srikanth Divi



Dr Jitendra Carpenter



Rishith Rajesh Khanna



Santusti Gour

Advisory Board

Mr. Bharat Muralidharan

Graduate of 2011 Batch, B.Tech. Chemical Engineering, MIT, Manipal.

M. S. Chemical Engineering, Rutgers University

Strategy Consultant – Deloitte USA

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Graduate of 2011 Batch, B.Tech. Chemical Engineering, MIT, Manipal.

Assistant Professor, Department of Chemical and Biomedical Engineering, West Virginia University, USA

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Graduate of 2012 Batch, B.Tech. Chemical Engineering, MIT, Manipal.

Postdoctoral Researcher, ChemSIN, Universite Libre de Bruxelles, Brussels, Belgium

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Ph.D., Leeds Univeristy, U.K.,

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Graduate of 1994 Batch, B.Tech. Chemical Engineering, MIT, Manipal.

(Adjunct Faculty, Dept. of Chemical Engineering, MIT, Manipal)

Director, Sahradaya College of Engineering & Technology, Trichur, Kerala.

Mr. Sandeep Kattamuri

Graduate of 2005 Batch, B.Tech. Chemical Engineering, MIT, Manipal.

M.S Chemical Engineering – Stanford, 2007

Strategic Advisor, Social Entrepreneur, Student of Law



 **Department of
Chemical Engineering**

**Academic Block 2,
Manipal Institute of Technology**

**Department of Chemical Engineering, Manipal Institute of Technology,
Manipal, Karnataka, India - 576104.**

Ph. No. +91 820 2924316 | Email: chemical@manipal.edu