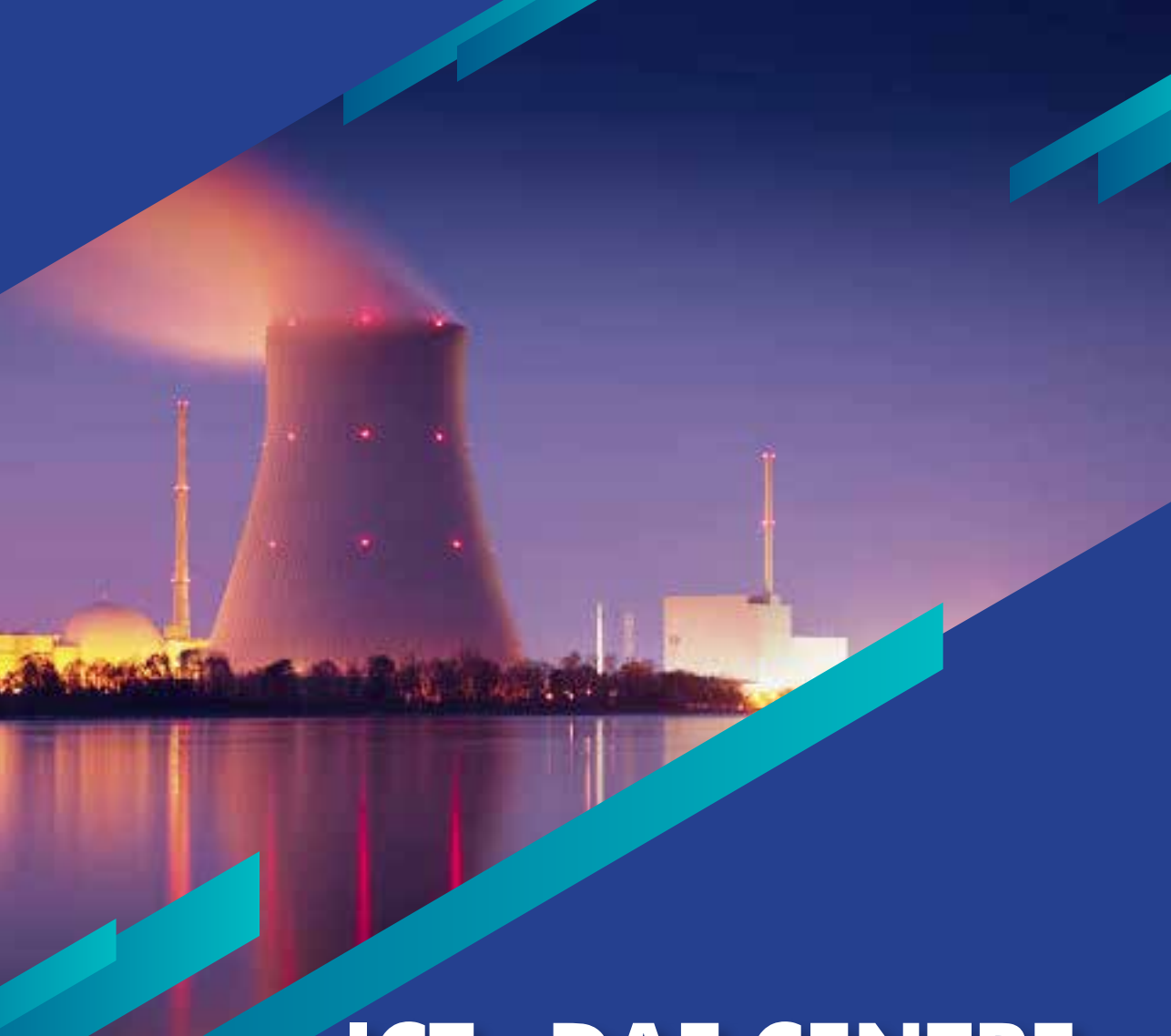


ICT–DAE CENTRE FOR CHEMICAL ENGINEERING EDUCATION AND RESEARCH

About DAE-ICT Center

The Institute of Chemical Technology (ICT) and the Department of Atomic Energy (DAE) instituted the ICT-DAE Centre for an interdisciplinary Ph.D. programme in Chemical Engineering to undertake R&D projects in the areas of common interest and related to nuclear, fuel cycle and advanced technologies. Under the Centre, the faculty members of the Departments of Chemical Engineering and Chemistry, collaborate with the DAE Research Institutions, namely, Bhabha Atomic Research Centre (BARC), Heavy Water Board (HWB) and Indira Gandhi Centre of Atomic Research (IGCAR) which are premier multidisciplinary R&D organizations engaged in research with the objective of generating knowledge and techniques for nuclear power production, advancement of science, use of radioisotopes in industry, health and agriculture as well as research in frontier areas of science and technology. BARC, HWB and IGCAR have pursued research and development in chemical engineering in a rigorous way for many years in the areas defined by DAE's mission oriented programmes as well as projects of national interest.

DAE has to develop several innovative technologies to tackle the problems of efficient nuclear fuel utilisation in the second and third stages of nuclear power programme. This requires a pool of qualified, motivated and talented young research scientists with multidisciplinary expertise. The number of Ph.D. level chemical engineers is small in this country and the number of chemical engineers entering DAE is even less. To satisfy the need of greater number of Ph.D. scholars well versed in basic sciences and chemical engineering, DAE and ICT have taken this initiative for imparting doctoral education in chemical engineering with multidisciplinary character through the ICT- DAE Centre.

ICT-DAE Centre supports a interdisciplinary PhD programme with candidates students drawn from Chemical Engineering, Metallurgical and Mechanical Engineering disciplines at the Bachelors and Masters Levels, and also from Chemistry, Physics, Biology and Mathematics streams with Masters degree. The Masters Degree holders in Engineering spend a minimum duration of 3 years, the Bachelors degree holder in Engineering 4 years and M.Sc. degree holder in science stream 5 years for earning the Ph.D. degree. The students are selected on the basis of all India written test and interview conducted jointly by ICT and DAE.

The Ph.D. scholars take up research projects primarily defined by BARC and IGCAR. However, there will be a certain degree of flexibility for selecting research projects outside the areas of relevance to DAE.

PROJECTS WITH ICT-DAE CENTRE IN COLLABORATION WITH BARC AND IGCAR

	Project Title	Principal Investigator	Principal Collaborator	Targets
1	CFD Modeling Asymmetric Rotating Disc Contactors	Dr. A.W. Patwardhan aw.patwardhan@ictmumbai.edu.in	S.K. Nayak S. O. / H	Design and experiments on 12 inch column, Sensitivity and Optimization of Geometry
2	Synthesis and modification of carbon nanotubes : modeling, experimentation and application	Prof. J.B. joshi jb.joshi@ictmumbai.edu.in	Dr. Kinshuk Dasgupta kdg@barc.gov.in	5% and 1% N and B doped CNT @ g/hr scale, Effect of parameters and kinetics, Aerogel kinetics and demonstration, Post synthesis modifications - noble metal loading, 3% by weight H2 storage, kinetics of H2 adsorption
3	Development of grafted memberanes (extractants) for radioactive and other metals	Dr. Anand V. Patwardhan av.patwardhan@ictmumbai.edu.in	Dr. Prasanta kumar Mohapatra	Synthesis of ligand functionalized resins and membranes, Loading studies on resins and membranes, Modeling studies, Delivering loaded resins and membranes to BARC, Actual Waste studies in BARC
4	Conjugation and radiolabeling of various nanoplatoforms for image guided theranosti applications	Dr. R.D. Jain rd.jain@ictmumbai.edu.in	Dr. Rubel Chakravarty rubelchakravarty@gmail.com Dr. Sudipta Chakraborty sudipta@barc.gov.in	Rapid and scaleable method for polymeric and metallic NP, Radiolabelled Silver NP, Validation through Fluorescent labeling, Proof of bio activity
5	Electrochemical behavior of uranium(III), Zirconium(IV) and aluminium(III) present in room temperature ionic liquids	Prof. B.M. Bhanage bm.bhanage@ictmumbai.edu.in	Shri K.A. Venkatesan, FChD, CG 24082/24287 kavenkat@igcar.gov.in	Ionic liquid suitable for electrochemical studies, Dissolution and Electrochemical behaviour of U, Zr, Al, Metal deposition and electrowinning from IL,
6	Synthesis of N,N-dialkyl-2-alkoxyacetamides extractants and N,N-dialkyl-2-alkoxyacetamides grafted resins for the separation of trivalent actinides from nitric acid medium and modeling of extractants.	Prof. Radha V. Jayaram rv.jayaram@gmail.com	Shri K.A. Venkatesan, FChD, CG 24082/24287 kavenkat@igcar.gov.in Dr.M.P.Antony	Synthesis of dialkyl-alkoxyacetamide derivatives, studies on HLW, Synthesis of loaded PS-DVB resins, Extraction behavior and column studies of Am and Eu resin, Understanding by QM-MM calculations

7	Improved process for CaSO4 crystallization in concentrated brine using ultrasound	Dr. Parag Gogate pr.gogate@ ictmumbai.edu.in	Abhijit Raha & Saurabh, Desalination Division, BARC	Understanding CaSO4 crystallization and Thermodynamic modeling, Effect of seeding on CaSO4 crystallization, Evaluation of direct/Indirect ultrasound assisted direct /indirect CaSO4 crystallization, scale-up strategies
8	Graphene based high-performance material for water desalination	Dr. Neetu Jha nr.jha@ictmumbai.edu.in	Dr. Soumitra Kar SO/F, MDS, ChEG, BARC	Synthesis and characterization of graphene and derivatives, Synthesis and characterization of electrodes and membranes, Testing for Water desalination
9	High Performance Laser – Process Development Design and Synthesis	Dr. N. Sekar n.sekar@ictmumbai.edu.in	Dr. Alok K. Ray, Head, Tunable Laser Section, L&PTD, BARC	Synthesis of Pyrrimethene 597 dye (50g), Cyano derivative of PM 597 (25 g), Synthesis of new red shifted PM dye (20g), High Purity PM567 Dye (50 g), Synthesis of Phenalemine 512 laser Dye (2g)
10	Development of experimental setup for production of monodiperse microsphere	Dr. R.D. Jain rd.jain@ictmumbai.edu.in	Dr. K. Ananthasivan FChD, CG, OGCAR asivan@igcar.gov.in Intercom : 24069 9445307229	Experimental setup for production of 2800 & 500 μm monodiperse microspheres March -2020
11	Bioenhanced & Targeted Drug Delivery System Of Deuterated Mitocurcumin	Prof. P. V. Devarajan, pv.devarajan@ ictmumbai.edu.in	S. Santosh Kumar, RB&HSD, BARC	Synthesis, Characterization and Analytical Method Development of Mitocurcumin, Metabolism studies on mitocurcumin, Preformulation study, Development and optimization of Nano drug delivery system of mitocurcumin, PK and Biodistribution studies of Nano drug delivery system of mitocurcumin,
12	Modified Deuterated Polyphenols As Chemotherapeutic And Antimicrobial Agents	Prof. M. S. Degani, ms.degani@ ictmumbai.edu.in	Kshama Kundu , S. Santosh Kumar, RB&HSD, BARC	Synthesis of triphenyl phosphine derivatives of polyphenols (Mito-Polyphenols) and Deuteration of Mito-polyphenol, Screening of synthesized triphenyl phosphine derivatives for enhanced anti-bacterial activity, Metabolism and toxicity studies of synthesized derivatives
13	Modified novel deuterated amino acids and small molecules for possible increase of lifetime of an active drug	Prof. S. V. Joshi, sv.joshi@ictmumbai.edu.in	D. Goswami, BARC, Ananya Verma HWB	Synthesis of 5-Bromo Tryptophan (Bromo compound) which is the key starting compound for synthesis of ‘deuterated amino acids’
14	Extraction and Deuteration of Natural Products of Therapeutic Importance for Improved Potency	Prof. K. S. Laddha, ks.laddha@ ictmumbai.edu.in	D. Goswami, BARC	Extraction , isolation and characterization of Artemisinin from Artemesia annua.

Ph.D. SCHOLARS (CURRENT) UNDER ICT-DAE CENTRE OF CHEMICAL ENGINEERING EDUCATION

Sr.	Name	Title of Ph.D. Project	Previous Institute	Qualification	Supervisor
1.	Bhavesh Gajbhiye	Thermal hydraulic studies related to coolants for new generation reactants	ICT, Mumbai	M. Chem. Engg.	Dr. C. S. Mathpati
2.	Sandeep Gosavi	Computational fluid dynamics and experimental study of fluidization of Li-Ti particles in fluidized and packed fluidized bed	ICT, Mumbai	M. Tech.	Dr. C. S. Mathpati
3.	Zakir Hussain	Modelling and simulation of solid fuel burning devices	UDCT, Jalgaon	M. Tech.	Prof. A. B. Pandit
4.	Rajput Swapnil K	Development of grafted resins and membranes (extractants) for precious metals	ICT, Mumbai	M.Chem. Engg.	Prof. Anand V. Patwardhan
5.	Tiwari Shashank S.	Transport Phenomenon in Gas- Solid Systems	NIT, Bhopal	M.Tech.	Prof. A.W Patwardhan.
6.	Gaikwad Ganesh	Conjugation and radiolabeling of various nanoplatforms for image guided theranostic applications	UDCT, Jalgaon	M.Tech.	Prof. V.G. Gaikar
7.	Hendre Nilesh V.	CFD Modeling of Asymmetric Rotating Disc Contactors	NIT, Trichy	M.Tech.	Prof. A. V. Patwardhan
8.	Shruti Hinge	Computational fluid dynamics of the stirred reactors	ICT, Mumbai	M.Chem. Engg	Prof.A.W. Patwardhan
9.	Pratiksha Madhukar Biranje	Synthesis and modification of carbon nanotubes modelling experimentation and applications	ICT, Mumbai	M.Tech. (Oils)	Prof.A.W. Patwardhan
10.	Amol Vilas Ganjare	Development of grafted membranes (extractants) for radioactive and other metals.	ICT, Mumbai	M.Tech (Oils)	Prof.A.V. Patwardhan
11.	Shrilekha Vijaysinh Sawant	Synthesis and modification of Carbon nanotubes: Modeling, Experimentation and Applications	ICT, Mumbai	M.Tech. Green Technology	Prof .J.B. Joshi

12.	Tukaram Udhavrao Shinde	Mathematical modelin of the Gas centrifugal separator	LIT, Nagpur	M.Tech.	Dr. V.H. Dalvi
13.	Sarvesh Sanjay Sabnis	Improved Separations and Cleaning Using Ultrasound	ICT, Mumbai	M.Tech.	Dr. Parag R. Gogate
14.	Vikram Vijay Banakar	Improved process for CaSO4 crystallization in concentrated brine Using Ultrasound	UDCT, Jalgaon	M.Tech.	Dr. Parag R. Gogate
15.	Vaishnavi Pabbisetty	Graphene based high performance materials for desalination	ICT, Mumbai	M.Chem. Engg.	Dr. Parag Nemade
16.	Chaitanya Dileep Moholkar	Improved process for CaSO4 crystallization in Concentrated brine using ultrasound – CFD Modeling	AISSMS, Pune	M.Tech.	Prof. P. R. Gogate
17.	Shreerang Dattatray Datar	Graphene based high performance materials for water desalination	ICT, Mumbai	M.Tech. Green Technology	Dr. Neetu Jha
18	Dhruti Rakte	Graphene based high performance material for water desalination	ICT, Mumbai	M.Chem. Engg.	Dr. Parag Nemade
19.	Momin Rahat Farooque Ahmed	Improvements in membrane separation using ultrasound	Bharati Vidyapeeth, Pune	M.Tech.	Dr.Parag Gogate
20.	Rutuja S. Bhoje	Graphene based membrane separation	Dr. Babasaheb Ambedakar Technological University, Lonere	M.Tech.	Dr. P. R. Nemade
21.	Satyajeet Yadav	Development of hydrodynamic flow focusing droplet generator for preparation of mono-disperse actinide oxide microsphere	Bharti vidyapeeth college of engineering, Pune	M.Tech. Chemical Engineering	Prof. A.B. Pandit
22.	Bhujbal Akshay Vilas	Electrochemical behaviour of U (III), Al (III) and Zr (IV) in Ionic liquid medium	Savitribai Phule Pune University, Ganeshkhind, Pune	M.Sc. in Organic Chemistry	Prof. Bhalchandra M. Bhanage
23.	Esha Attar	Bioenhanced and targeted drug delivery system of deuterated mitocurcumin	Sinhgad College of Pharmacy, Vadgaon(Bk), Pune.	M.Pharm (Pharmaceutics)	Prof. P. V. Devrajan
24.	Vishakha Likhite	Bioenhanced and targeted drug delivery system of deuterated mitocurcumin	Bombay College of Pharmacy, Kalina. Mumbai.	M.Pharm (Pharmaceutical Chemistry)	Prof.P.V. Devrajan

25.	Kranti Kamble	Extraction and Deuteration of Natural Products of Therapeutic Importance for Improved Potency	C.U.Shah College of Pharmacy, S.N.D.T. Woman's University	M.Pharm (Quality Assurance)	Prof K. S. Laddha
26.	Ashwini Patil	Modified deuterated polyphenols as chemotherapeutic and antimicrobial agents	R. C. Patel Institute of Pharmaceutical Education & Research. Shirpur. Dhule	M.Pharm (Pharmacology)	Prof. M.S.Degani
27.	Mahin K.I	Modified deuterated polyphenols as chemotherapeutic and antimicrobial agents	Institute for Integrated programmes and Research in Basic Sciences (IIRBS),Mahatma Gandhi University, Kerala	M.Sc (Chemistry)	Prof. M.S.Degani
28.	Sandeep Avadutha	Deuterated Amino Acids for Possible Increase of Lifetime of an Active Drug	D.G.Ruparel College, Mahim	M.Sc (Chemistry)	Prof. S.V.Joshi
29.	Sumeet Sonvane	High Performance Laser Dyes Design and Synthesis	Department of Chemistry, Dr. Babasaheb Ambedakar Marathwada University, Aurangbad	M.Sc. (Organic Chemistry)	Prof. N. Sekar
30.	Amid Sadgar	Synthesis of N,N-dialkyl-2-alkoxyacetamides extractants and N,N- dialkyl-2-alkoxyacetamide grafted resins for the separation of trivalent actinides from nitric acid medium and modeling of extractants	ICT, Mumbai	M.Tech (Green Technology)	Prof. R.V. Jayaram

LIST OF STUDENTS COMPLETED Ph.D. UNDER ICT-DAE CENTRE OF CHEMICAL ENGINEERING EDUCATION

Sr.	Name	Title of Ph.D. Thesis	Supervisor
1.	Meena Singh	Molecular dynamic Studies of Metal ions & their Complexes	Prof. V.G. Gaikar
2.	Hrushikesh Khadamkar	Studies in liquid-liquid extraction: Marangoni convection	Prof. A. W. Patwardhan
3.	Pravin Bote	Novel reactor design for synthesis of different oleochemicals	Prof. V.G. Gaikar
4.	Anita Sharma	Synthesis of carbon nanotubes	Prof. A. W. Patwardhan
5.	Swapnil Chaudhari	Transport of actinides and fission products across hollow fibre supported liquid membranes	Prof. A. V. Patwardhan
6.	Vishal Sawant	Design and synthesis of extractant for selective extraction of metal ions from nuclear Waste	Prof. V.G. Gaikar

Research Student: Bhavesh D. Gajbhiye

Project Title:	Thermal hydraulic studies related to coolants for new generation reactors.	
Supervisor from ICT:	Dr. C. S. Mathpati Associate Professor, Institute of Chemical Technology, Mumbai	
Co-Investigator:	Prof. A. W. Patwardhan Head of the Chemical Engineering Department, Institute of Chemical Technology, Mumbai	

Highlights of the Work:

In order to develop design strategies for coolant system of high temperature new generation nuclear reactors, the current work aims to test the thermal hydraulic characteristics of different coolants operating at high temperatures. Based on the previous work in this area, molten fluoride salt FLiNaK was found to be the most suitable coolant and heat transfer media at high temperatures (500 to 1450 °C). It can be concluded from the reported literature that an extensive research for coolants corrosion properties and heat transfer characteristics is required. Thus, based on the analysis from the literature review for the design of Generation-IV nuclear reactors the major challenges were identified and experiments were planned accordingly. The material corrosion analysis in molten FLiNaK salt was carried out at high temperatures (650 to 850 °C) and the results are reported in our previous work. Based on the corrosion information, a high temperature forced convection loop for experimental thermal hydraulic studies of the extremely corrosive molten fluoride salts was designed and fabricated. To develop safe experimental procedures and reduce the risk by identifying and minimizing potential hazards before carrying out experiments with extremely corrosive fluoride salts at very high temperatures, pre-tests were carried out using simulant thermic fluid Thermia-B (at 100 – 200 °C) and water (at 30 – 100 °C). Heat transfer was found to increase with respect to Reynolds number in all the different cases of heat input to the test section and was well correlated with the empirical correlations. The set-up provides vital information for thermal hydraulic design of the heat transfer circuit in high temperature molten salt nuclear reactor technology.

Research Student: Sandeep Namdeo Gosavi

Project Title:	Computational Fluid Dynamics and Experimental study of Fluidization of lithium Titanate particles in fluidized and packed Fluidized bed	
Supervisor from ICT:	Dr. C.S. Mathpati, Associate Professor, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai	
Co-Investigator:	Dr. D. Mandal, Head, AMMD, Chemical Engineering Divison, Bhabha Atomic Research Centre, Mumbai	

The imitation of fusion process happening on the Sun in controlled manner is challenging task and if successful, will provide with practically unending source of energy. One of the problem lies in efficient transport of the heat generated in the core of the reactor. We are working on development of Packed Fluidization systems which try to remove heat generated in most efficient way. Fine particles are fluidized in interstitial spaces so that the attributes of both packed bed and fluidized bed can be incorporated in single continuously operated system.

Work done:

- Analysis of different packing algorithm to generate packed bed geometry
- CFD Simulations to predict the effective thermal conductivity Packed Bed
- CFD simulations to predict Minimum Fluidization Velocity in Packed Fluidized Bed

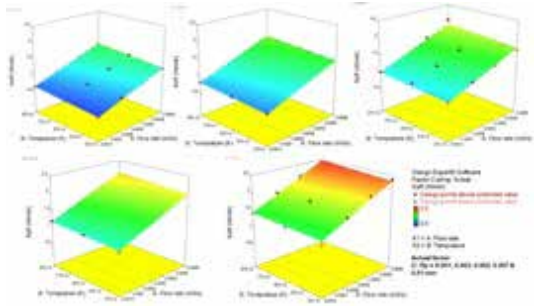


Figure: Response surface for effect of particle size on Keff at different flow rate and wall temperature

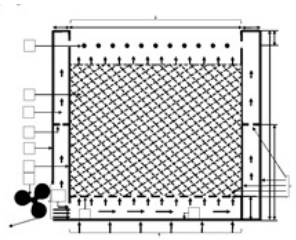
Different packing algorithms to generate the random 3D packed bed geometry are compared in this section. The suitability of such predicted bed configurations for subsequent study by CFD simulations is tested. Heat transfer simulations. CFD simulations were performed to predict the effective thermal conductivity in packed beds and the predictions were within 10% of the experimental observations. Subsequently the CFD simulations were done for prediction of minimum fluidization velocity in packed fluidized beds. The modeling results are promising and can be extended to further to heat transfer studies in packed fluidized beds.

Research Student: Zakir Husain Mohammed Yusuf

Project Title:	Modeling and Simulation of Solid Fuel Burning Device	
Supervisor from ICT:	Prof. A. B. Pandit, Institute of Chemical Technology, Mumbai	
Co-Investigator:	Prof. J. B. Joshi, Emeritus Professor, ICT, Mumbai	

Highlights of the Work Done:

CFD simulations were performed to investigate the fluid phase hydrodynamics, homogenous and heterogeneous combustion in a biomass cook-stove (BCS). An optimization study has been carried out to investigate the effective air distribution through biomass cook-stove. In order to improve the air distribution uniformity, a wide range of velocities were used to predict the effect of secondary air inlet orifices, support grate, and packing on air flow quality of BCS. An increase in the uniformity index of around 6.5 % was observed with a proper configuration of



orifice and grate plate combination. Gas phase simulation shows non-obvious evidence of the linear dependence of power and temperature on the air velocity and air-fuel ratio. The understanding of hydrodynamic and homogeneous combustion was used to extend the simulation of the heterogeneous combustion in BCS. Further, batch pyrolysis of biomass pellets (agro and garden waste) was carried out over a temperature range of 200°C-600°C which generates mainly CO2, CO, H2 gases along with C1-C3 hydrocarbons at 600°C. The yield of non-condensable gasses, liquid products and bio char was 30 wt. %, 38 wt. %, and 32 wt. %, respectively. The mass spectroscopic analysis of the bio-oil depicted the presence of light oxygenates, furans, anhydrosugars, and phenolic compounds. A kinetic study of thermal decomposition of biomass pellets was performed. A reaction mechanism of the product formation during the pyrolysis was also purposed. The calculation of NER shows that the present system of biomass pyrolysis can be self-sustainable and is in fact energy surplus.

Research Student: Swapnil Rajput

Project :	Development of grafted resins and membranes (extractants) for precious metals
Supervisor from ICT :	Prof. Anand V. Patwardhan, Chemical Engineering Department, Institute of Chemical Technology, Mumbai

Diglycolamides are better choice for Actinide separations. But, there are some difficulties like high cost of production, inefficiency in high acidity and partition coefficients are low per unit mole. To overcome this issue, grafting of similar functionality over inert polymeric support has been used. Merrifield resin was chosen as inert polymeric support, over which different combinations based on alkyl chain length of diglycolamide functionalities (total 9) were grafted using 5-step reactions, wherein each reaction was optimized to improve grafting yield and easy unit operations as they are going to affect scale-up of technology. Once, the 5-steps are fully optimized in terms of yield and usage of as less excess reagents as possible (which is a curse in polymer chemistry), different specifications of same resin were tried. A 200-400 mesh sized 1.8mmol of Cl/g of resins gave Kd values in the range of 20-225 ml/g, which were not good enough for target Kd values. Thus, resin of 16-50 mesh sized with 5.5mmol Cl/g of resins gave Kd in range of 1150-5500 ml/g for preliminary experiments, which not only met our target Kd value. The grafting reactions were altered to get more surface area as larger resins were facing uptake issues because of low surface area to volume ratio. The scale up of process is completed to regulate engineering parameters which might affect the final grain size. and MRBB (Merrifield Butyl-Butyl diglycolamide derivative) is chosen as best resin out of synthesized 9 resins and it's mechanism of uptake was confirmed by mathematical modeling over GROMACS. Uptake study with surrogate metal ions under varied parameters is under way to find the optimum working conditions with desired size of synthesized resins.

Research Student: Shashank Surendra Tiwari

Project Title:	Direct Numerical Simulation of Flow Patterns in Multiparticle Systems
Supervisor from ICT:	Prof. Ashwin Patwardhan, Depart. of Chem. Engg. ICT Mumbai
Co-Investigator:	Prof. Jyeshtharaj B. Joshi, Emeritus Professor of Eminence, Depart. of Chem.Engg. ICT Mumbai

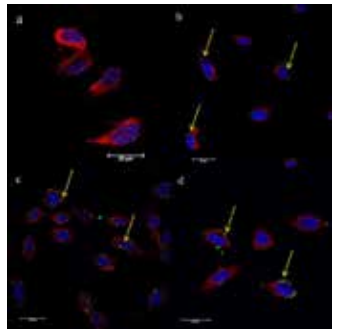
Fully resolved Direct Numerical Simulation (DNS) have been performed for highly turbulent free shear flows (Re > 104) for the first time.

- Statistical convergence studies have been performed to test the degree of accuracy of the data using second order discretization schemes in time and space.
- The length and time scales of the turbulent structures obtained from the three-dimensional velocity data have been estimated by relating them with the Kolmogorov length scale.
- A benchmark study is currently being performed by testing various combinations of domain sizes, mesh sizes, time step sizes and discretization schemes to develop basic guidelines for carrying out space resolved DNS using FVM.

Figure: Velocity iso-contours for flow past a sphere obtained from fully resolved DNS implemented on a hexahedral mesh configuration of 128 Million cells, using a second order accurate central differencing scheme.

Research Student: Mr. Gaikwad Ganesh Arjun

Project Title:	Conjugation and radiolabeling of various nanoplatforms for image guided theranostic applications
Principle Investigator:	Dr. R. D. Jain, UGC Assistant Professor in Engineering sciences, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai
Principle Collaborator:	Dr. Rubel Chakravarty, Radiochemical Section, Isotope Production and Application Division, Bhabha Atomic Research Centre Trombay, Mumbai
Principle Collaborator:	Dr. Sudipta Chakravarty, Radiochemical Section, Isotope Production and Application Division Bhabha Atomic Research Centre Trombay, Mumbai

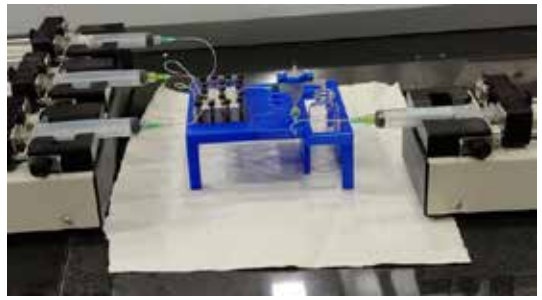


Part A: Continuous synthesis of Trimethyl chitosan/Palladium nanoparticles for potential anti-cancer therapy.

Trimethylated chitosan coated palladium nanoparticle synthesis using fabricated droplet microreactor has been successfully carried out. Cellular uptake and toxicity studies for palladium nanoparticles have been conducted. The result showed that the developed nanoparticles have ability to interact with cell membrane and internalize within the cell body.

Figure1: Confocal studies for palladium nanoparticles using MCF-7 (breast cancer) cell line of a) Control (without nanoparticle) and b) 10 µl c) 20 µl d) 30 µl FTIC labeled TMC coated Pd NPs.

The photo-thermal property of Pd nanoparticles for assessing their potential as theranostic agent has been carried out for cancer treatment application. Effect on temperature with respect to time and volume of nanoparticles were estimated prior to cellular studies. Maximum temperature of 63°C was achieved with volume of 100ul TMC/Pd NPs after exposure for 2 min. Cellular Photo-thermal Studies with Palladium Nanoparticles were performed on MCF 7 breast cancer cell line. The cell death rate was recorded as >90% at the optimum temperature condition of 55°C which was achieved with 25ul TMC/Pd NPs after exposure for 3 min using 1 W cm−2 808 nm IR laser. The TMC coated Pd NPs have potential as nano-therapeutic agent for enhanced therapy of tumors using a non-invasive near-infrared laser.



Part B: Radiolabeled Chitosan nanoparticles for cancer diagnosis. Intrinsically radiolabeled chitosan nanoparticles were successfully synthesized with Lu-177, Sm-153 and Ga-68 isotopes. Moreover, Cellular uptake and toxicity studies for Chitosan-Lu nanoparticles have been conducted which shows good uptake of nanoparticles in cells.

Figure2: Experimental setup for Palladium nanoparticle synthesis

Research Student: Nilesh Virbhadra Hendre

Project Title:	Computational fluid dynamics study of Asymmetric rotating disc contactors
Supervisor from ICT:	Prof. A. W. Patwardhan Institute of Chemical Technology, Mumbai
Co-Investigator:	Dr. S. K. Naya, Heavy Water Board, Mumbai

12" ARIC

Highlights:

Hydrodynamic performance of laboratory scale (4" I.D) and pilot scale (12" I.D) asymmetric rotating impeller column (ARIC) was investigated over a range of wide operating conditions and throughputs. Decrease in drop size and increase in dispersed phase holdup was observed with increase in impeller speed in both the columns. Mass transfer performance of pilot scale ARIC was found to be satisfactory. The height of transfer unit was observed to be 0.7 m and number of transfer units close to 3. Furthermore, computational fluid dynamics (CFD) simulations coupled with population balance modeling (PBM) for ARIC were carried out. The breakage and coalescence model of Coulaloglou & Tavlarides and Prince & Blanch were used, respectively. The drag model of Kumar and Hartland was employed for calculation of drag coefficient. The average error in prediction of both drop size and holdup was well within 10 %. CFD simulations also revealed regions of high turbulent energy dissipation rate which are present near impeller blades where drop size is observed to be minimum. This study will be useful during scale up to optimize different geometrical parameters to improve the efficiency of ARIC.

Research Student:	Shruti Hinge
Project Title:	CFD Modelling of Gas-Liquid Stirred Tank Reactors And Fermenters
Research Supervisor:	Prof. A. W. Patwardhan, Chemical Engineering Department, ICT

Computational fluid dynamics is a useful tool to design stirred tank reactors and fermenters and improve its performance using mathematical and computational modeling method. Present work deals with the CFD simulations of the stirred tank reactor with Newtonian and non-Newtonian fluids. For the experimental studies, water and an aqueous solution of carboxymethyl cellulose (CMC) are considered as model fluid with Newtonian and non-Newtonian behavior, respectively and air is considered as a gas phase. The experimental setup is shown in Fig 1. Studies have been carried out to identify the regime transition with 6-blade Rushton turbine for various gas flow velocity. The rheological properties of the CMC solution (0.1, 0.3, 0.5 and 0.7 %) have been measured with cone and plate viscometer. The effect of impeller speed, gas flow velocity and concentration of CMC on bubble diameter, local gas holdup and overall gas holdup have been studied. CFD model has been developed using Fluent 18.0 for given experimental setup. In order to validate the model, single phase simulations have been performed and velocity profiles have been compared with the data reported in previous studies by Joshi et al. (2011) and Khapre and Munshi (2015) for Newtonian and non-Newtonian fluids, respectively. The contours plots of tangential velocity for different rheological parameters (K and n) are shown in fig 2. The two phase simulations will be carried out and validated with the experimentally obtained holdup.

Fig 1. Experimental setup of the stirred tank reactor (6-blade Rushton turbine)

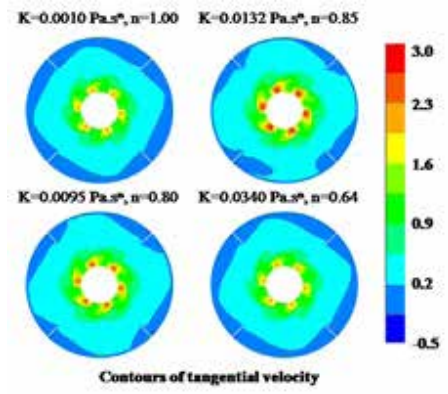


Fig 2. Contours plots of the tangential velocity plotted on the XZ plane (6-blade Rushton turbine)

Research Student: Ms. Pratiksha Madhukar Biranje

Project Title:	Synthesis and modification of carbon nanotubes: modeling, experimentation and applications	
Supervisor from ICT:	Prof. A. W. Patwardhan, Department of Chemical Engineering Institute of Chemical Technology, Mumbai	
Co-Investigator:	Prof. J. B. Joshi	

Graphene oxide(GO), a chemical derivative of graphene was successfully synthesized by electrochemical exfoliation of graphite.

A novel graphite electrode geometry used, have shown advantage of controlled layer by layer graphite exfoliation and re-exfoliation.

In electrochemical exfoliation route, electrolyte properties, density of graphite source, applied bias, temperature were shown to have direct effect on graphene oxide.

TEM analysis showed presence of narrow distribution in few layer graphene oxide sheets.

XPS showed that, graphene was loaded with different oxygen containing functional groups and was supported by Raman spectroscopic analysis by appearance of D-peak along with G and 2D.

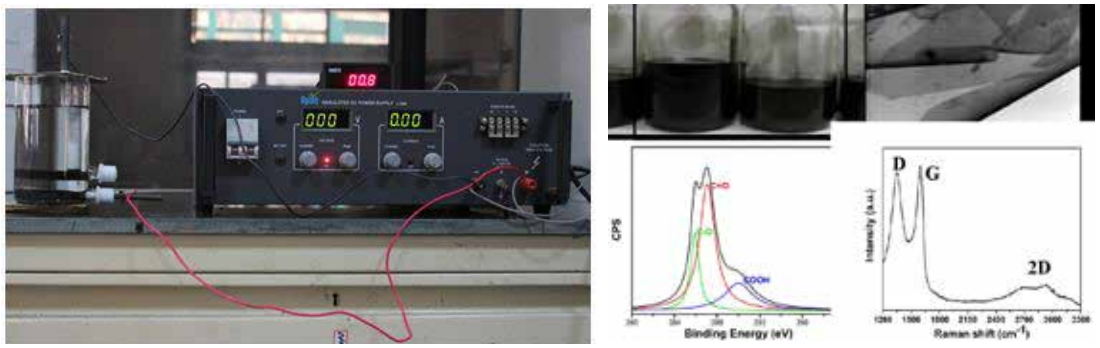


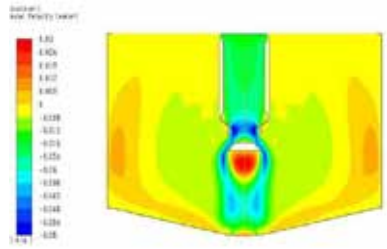
Fig. 1 (a) shows experimental setup, (b) GO dispersed in ethanol solution,(c)TEM image of GO,(d) XPS spectra of GO and (e) Raman spectra of GO.

Research Student: Amol Vilas Ganjare

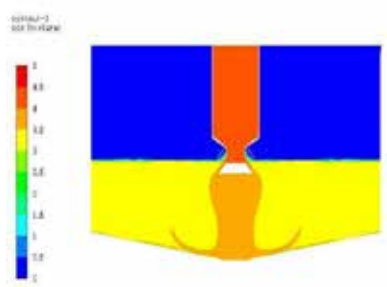
Project Title:	Design Aspects of Gravity Settlers	
Research Supervisor:	Prof. A. W. Patwardhan, Institute of Chemical Technology, Mumbai	

Sedimentation tanks are important part of the wastewater treatment plant. The gravity settling is efficient and cheaper way to separate suspended solids from water. The properties of the feed to the sedimentation tank affect the separation efficiency of sedimentation tank. In this study, sedimentation tank is studied for the particle settling behavior with computational fluid dynamics (CFD) by using Eulerian-Eulerian model. The study focused on the developing a CFD model for circular sedimentation tank. The CFD model for single-phase and two-phase flow in the settlers is developed. Selection of the turbulence model along with drag laws and various operating conditions is studied. It is noticed that, the low RE turbulence model preformed well as compared to standard k-epsilon model. Lab scale experimental facility is developed. The settling behavior in the continuous operation of the settler is studied. Two-dimensional axisymmetric model was considered for CFD study. The grid dependency to results was studied with different grids. The study focused on the effect of different particle density on the flow field and the particle distribution in the settling tank. The particle density varying from 1200-2500 kg/m3 is considered. The solid concentration in the feed was kept at 4% and flow rate was 30 LPH in all the studied cases. Two outlets of the sedimentation tank were kept at equal flow rate. The aim of the study is to achieve optimize operating conditions for maximum separation efficiency.

Experimental Setup: Continuous gravity settling



Contours of Axial Velocity



Concentration distribution for Density= 2500kg/m3

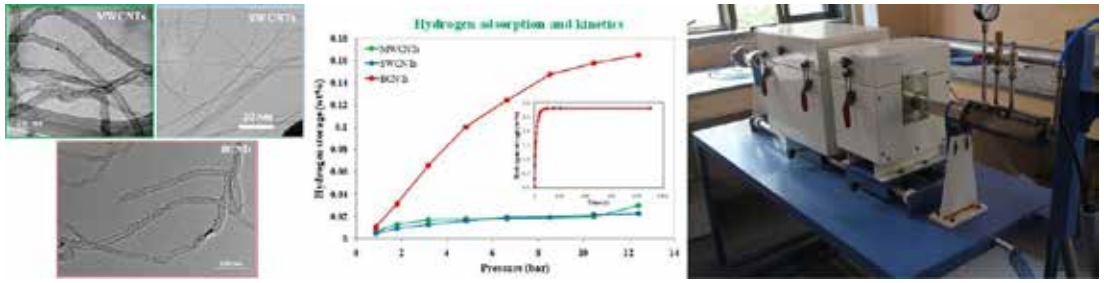
Research Student: Shrilekha Vijaysinh Sawant

Project Title:	Modification of Carbon Nanotubes; Synthesis, Characterization and Applications	
Supervisor from ICT:	Prof. A. W. Patwardhan, Institute of Chemical Technology, Mumbai	
Co-Investigator:	Prof. J. B. Joshi, Institute of Chemical Technology, Mumbai Dr. Kinshuk Dasgupta, Bhabha Atomic Research Center, Mumbai	

Highlights:

Floating catalyst chemical vapor deposition (FCCVD) method was used for synthesis of boron doped carbon nanotubes (BCNTs) using ethanol, triethyl borate and ferrocene as carbon, boron and catalyst precursor respectively. The hydrogen adsorption activity was studied for BCNTs along with undoped single walled and multi walled carbon nanotubes (SWCNTs and MWCNTs). BCNTs were having 7 times higher hydrogen adsorption values than SWCNTs and MWCNTs. Hydrogen adsorption for BCNTs was found to be 2.5 wt% at 10 bar and 77K. Similarly, Boron, Nitrogen-doped CNTs (B, N-CNTs) were synthesized using ethanol, boric acid, imidazole and ferrocene as carbon, boron, nitrogen and catalyst precursor respectively. Hydrogen storage value reported for B, N-CNTs was 1.96 wt% at 10 bar and 77K.

Graphical abstract and Experimental setup:



Research Student: Tukaram Shinde

Project Title :	Heat transfer studied of the solar thermal systems: its experimentation, application and deployment
Research Supervisors:	Dr. Vishwanath H Dalvi, Assistant Professor, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai

The project is aimed to design, analyze, deployment, and optimization of solar thermal devices. The devices like thermal receivers, heat exchangers, collectors, thermal storage defined as the total effectiveness of the solar thermal systems. The efficiency depends upon the two parameters thermal and optical, so the thermal efficiency is a crucial factor to study and analyze. Thermal designs based on various models of conductive, convective, and radiation heat transfer models, but still, there is a necessity for the development of these models. There is still a gap between the development of models with combined models of optical and thermal energy.

The novel concept design of receiver (Thermal diode) tried to replace with conventional receiver for better heat efficiency. An experimental investigation is carried out of thermal diode receiver under real sun see fig 1. Application of solar thermal power carried out for poultry space heating, tackling the problem of brooding in the winter season, see fig. 2 for the actually developed prototype.

Figure 1: Thermal diode receiver experimentation under the sun.

Figure 2: Any source of heating (solar, wood, LPG gas) assisted poultry warmer developed for open poultry shed maintaining thermal comfort during winter in poultry shed.

Research Student: Sarvesh Sanjay Sabnis

Project Title:	Improved Crystallization and Cleaning Using Ultrasound (2018-19)
Supervisor from ICT:	Dr Parag R. Gogate, Department of Chemical Engineering, Institute of Chemical Technology Mumbai

Calcium sulphate ($CaSO_4$) is one of the sparingly soluble salts which tends to deposit on the heat exchange equipment during thermal desalination process. $CaSO_4$ is not a major component of seawater and its actual presence when investigated is found to be negligible. Even then, it causes difficulty in the operation of desalination plants because its formation is accelerated at higher temperatures by the reaction of sodium sulphate and calcium chloride whose concentrations are substantial (excluding sodium chloride). Therefore, formation of $CaSO_4$ from $Na2SO_4$ and $CaCl_2$ under different temperature conditions is studied. An ultrasound assisted approach is investigated so as to check the effect of acoustic cavitation on the induction time, yield, morphology and particle size of $CaSO_4$ in comparison to conventional method. There was a 10-20% reduction in the induction time with increased yield and about 25% reduction in the particle size with unimodal size distribution due to which separation becomes easier. This was also confirmed using microscopic analysis.

Also a commercial polymer additive (DADPS) was crystallized by antisolvent crystallization in presence of ultrasound. Size reduction of the additive is important for from the point of view of uniform dispersion in the host polymer. XRD and particle size measurement were used for characterization. About 85% size reduction was obtained without compromising on crystallinity (Fig 2). Scale-up prospects were also explored using an ultrasonic bath and these results were also promising.

Following schematic represents the ultrasound assisted size reduction of DADPS:

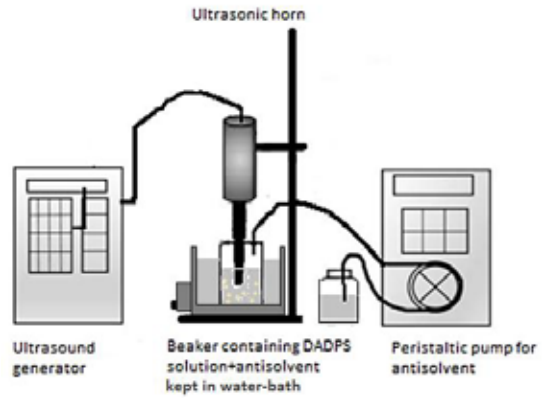


Figure 1: *Schematic representation of ultrasonic treatment for size reduction of DADPS in antisolvent crystallization*

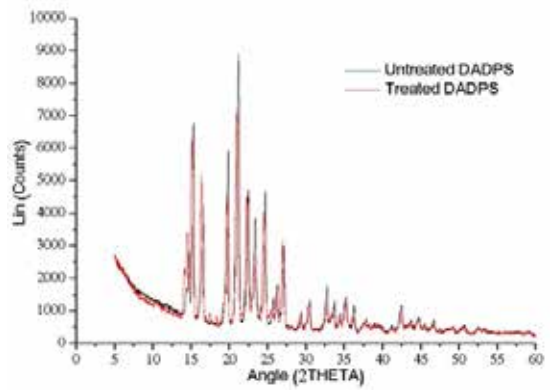


Figure 2: *XRD plot of untreated (black) and treated (red) DADPS*

Research Student:	Vikram Vijay Banakar
Project Title:	Improved process for $CaSO_4$ crystallization in concentrated brine Using Ultrasound
Supervisor from ICT:	Dr Parag R. Gogate, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai

Scaling is an important problem in the thermal desalination operation which is mainly attributed to the scale formation on the tubes due to the deposition of salts providing additional resistance to heat transfer. To reduce or prevent the formation of scale on heat transfer surfaces, treating desalination concentrates by precipitating sparingly soluble salts with ultrasound is a promising method. In the present work, the effect of ultrasonic pretreatment to the feed CaSO4 solution on the heat transfer rate has been investigated. For this study, lab scale double pipe heat exchanger setup was designed as shown in fig. 1 and operated under simulated conditions of the thermal desalination process. To understand the process of CaSO4 scaling initially, solutions of CaSO4 in DI water, NaCl solution and artificial seawater (ASTM D 1141-98) were prepared using determined solubility data of CaSO4 in respected solution as depicted in fig. 3 and used for scale deposition experiments. The experiments conducted using saturated CaSO4 solution in DI water and artificial seawater confirmed the scaling and drop in the heat transfer coefficient. A significant drop in the heat transfer coefficient was observed with lower value of 1.13 kW/m2.K (in first 10 h of operation) further reducing to 0.88 kW/m2.K at 50 h operation. SEM-EDX analysis was also performed to establish the morphology and main components of the scale (fig.2).

To reduce or prevent the formation of scale, CaSO4 solutions was irradiated with ultrasound to precipitate sparingly soluble $CaSO_4$ crystal. After crystallization, the crystals were separated and the solution was passed through the heat exchanger to check the effect on heat transfer rate. It was clearly demonstrated that the heat transfer rate was found to be higher than the previous case of untreated CaSO4 solution. To check the efficacy of seeding approach for scale control seeds were prepared by mixing equimolar concentration of Na2SO4 and CaCl2 at 70° C and analyzed using particle size analyzer for particle size distribution.

Fig 1: Modified setup with electrical heating and Condenser assembly to prevent evaporation

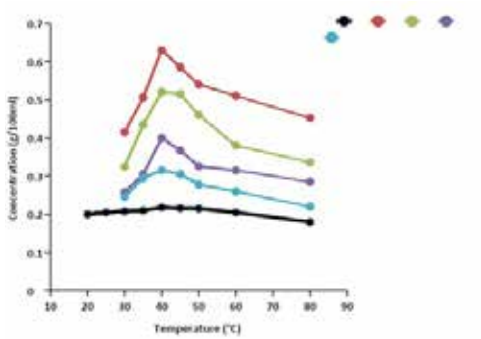


Fig 2: Comparison of solubility's of $CaSO_4$ in water and in different NaCl- water concentrations

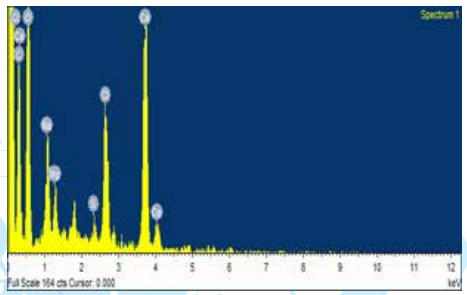


Fig 3: EDX of the formed scale

Research Student: Vaishnavi Pabbisetty

Project Title:	Graphene based high performance materials for desalination
Supervisor from ICT:	Dr. Parag. R. Nemade, Assistant Professor, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai
Co-Investigator:	Dr. Soumitra Kar, Scientific Officer F, Desalination Division, Bhabha Atomic Research Centre Trombay, Mumbai

The various properties of Graphene have led to its increased application. The increased application have necessitated the synthesis of Graphene based membranes at larger scale and at an optimal cost for the purpose of lowering the cost of recovery of potable water from saline solutions to address water shortages as well as to achieve zero discharge for industrial effluents.

Highlights:

- Synthesis of Thin film composite nanofiltration membrane.
- Checking the effect of polymer composition of the substrate on the performance of Thin Film composite nanofiltration membrane.
- Covalent binding of graphene oxide to thin film composite membrane(TFN).
- Performance studies (salt rejection and flux) of thin film composite (TFC) and thin film nano composite (TFN) membranes.
- Characterization of TFC and TFN.

Proposed Work:

- Optimization of composition of substrate of Thin Film Composite.
- Characterization of TFC and TFN.
- Fabrication of spiral module.
- Checking the performance of spiral module.

Nanofiltration test skid at Desalination Division, BARC

Research Student: Chaitanya Moholkar

Project Title:	Improved process for CaSO4 crystallization In concentrated brine Using Ultrasound: CFD Studies
Supervisor from ICT:	Dr. Parag R. Gogate, Department of Chemical Engineering, Institute of Chemical Technology Mumbai

CFD is an effective tool for simulating experimental set-ups to study the effects of various parameters and gaining additional valuable information for designing etc. Scaling is an important problem in the thermal desalination operation which is mainly attributed to the scale formation on the tubes due to the deposition of salts providing additional resistance to heat transfer. To reduce or prevent the formation of scale on heat transfer surfaces, treating desalination concentrates by precipitating sparingly soluble salts with ultrasound is a promising method. In the present work, the effect of ultrasonic pretreatment to the feed CaSO4 solution on the heat transfer rate has been investigated.

For this study, lab scale double pipe heat exchanger setup was designed. While experiments are performed on the set up, CFD simulation is done for the same and heat transfer is studied. ANSYS Fluent 16.0 is software used for simulation. Experimental and CFD results show congruence. CFD model is validating experimental findings. Results are shown in Table 1 and contour plots are shown in fig. 1. Small variation of CFD results from experimental results can be attributed to heat loss and experimental errors.

In order to generate acoustic cavitation, it was necessary to simulate the acoustic pressure waves in CFD. Separate CFD simulation is conducted to generate 2D Acoustic Pressure waves. ANSYS Fluent 16.0 is the software chosen in which the objective have been achieved by the combined use of User Defined Function (UDF) and Dynamic Meshing (Vibrating Grid). The profile contours and graphs are shown in fig. 3 and fig. 4 respectively.

Tube	Temperature	Annular Region	Temperature
T (in)	358.16 K	T(in)	320.16 K
T(out)-EXP	**345.16 K**	T(out)-EXP	**346.16 K**
T(out)-CFD	**348.62 K**	T(out)-CFD	**349.07 K**

Table 1: *Results - Double pipe Heat Exchanger : CFD vs Experiment*

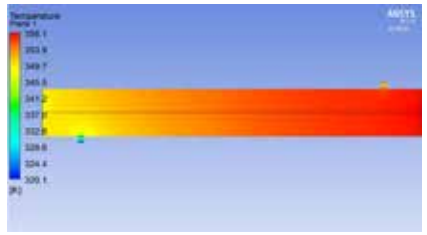


fig 1 : Temperature contours for Double Pipe Heat Exchanger

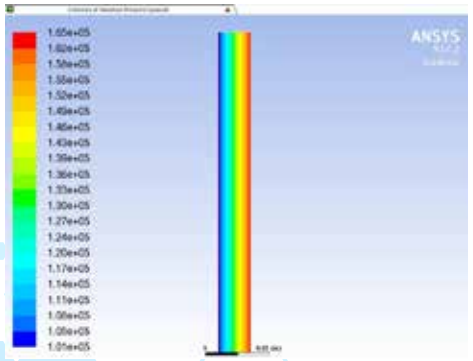


fig 2: *Acoustic pressure profiles Contours*

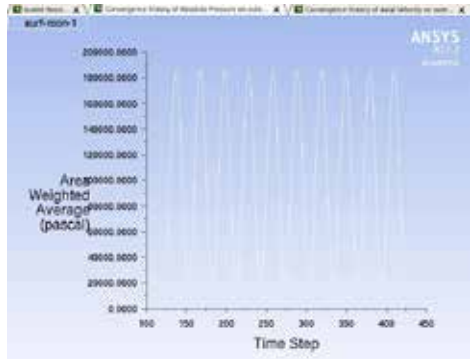
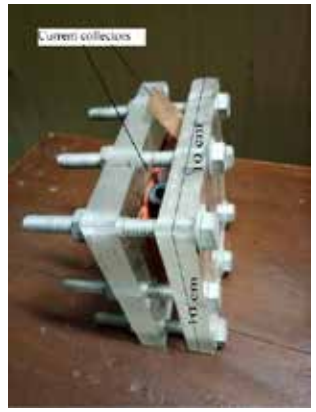


fig 3: *Sinusoidal pressure variation profile graph*

Research Student: Shreerang D. Datar

Project Title:	Graphene based high performance material for water desalination
Principal Investigator (PI):	Dr. Neetu Jha

Graphene oxide (GO) was prepared by Hummers' method. The as-prepared GO was reduced by using focused sunlight using convex lens. This reduced grapheme oxide termed as 'Solar reduced graphene oxide' (SrGO). The as-prepared SrGO was loaded on carbon paper by spin coating.



Flow-between capacitive deionization set-up was fabricated as shown in Figure. In the set-up, carbon papers were used as electrodes. The as-prepared SrGO was loaded on carbon paper by spin coating. Current collectors were made up of copper sheet. Whole assembly was stacked between two acrylic plates with the help of rubber gaskets as shown in Figure. Aqueous sodium chloride (NaCl) solution of different concentrations was used as the salt solution. Several voltages and salt concentrations were used at a time for carrying out desalination experiments. Effect of voltage and effect of salt concentration on electrosorption capacity in the set-up were studied. Further, the desalination experiments were carried out by using KCl as salt solution. Again effect of voltage and effect of salt concentration on electrosorption capacity were studied. It was observed that electrosorption capacity obtained for KCl is higher as compared to NaCl. This could be because of the difference in hydrated radius of two salts.

Research Student: Dhruti Rakte

Project Title:	Graphene based high performance material for water desalination
Supervisor:	Dr. Parag Nemade

Graphene oxide based thin film polyamide membranes were synthesized for desalination application. For the purpose, the GO is being synthesized in lab using various methods to control the oxidation content and size of the particles. Out of many methods tried, improved Hummers method is focused. This GO has been compared with commercially available GO [procured from Sigma Aldrich]. The lab synthesized GO proved to be far better with oxygen content than commercial GO. However, the particle size of lab synthesized GO was observed to be considerably larger.

The polyamide layer in which the (GO) is to be incorporated has thickness of about 0.2-0.3 micron. Hence it becomes imperative to synthesize GO that has particle size lesser than 200nm. Currently, experiments are being conducted to study effect of sonication and temperature on GO particle size without compromising the oxygen content.

Following is the Membrane crossflow filtration set up [a], graphene oxide synthesis set up [b] and maximum possible oxidation of graphite accordingly reported [c] respectively.



[a] [b] [c]

'Graphene oxide dispersed thin film composite membrane study' has been presented at The 6th IWA Regional Membrane Technology Conference (IWA-RMTC 2018) Vadodara on Dec 11th, 2018.

Research Student: Rahat F. Momin

Project Title:	Improvement in Membrane Separation using Ultrasound	
Supervisor from ICT:	Dr. P. R. Gogate, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai	

Membranes are of immense importance in industrial separation processes and are extensively used in a wide range of applications including desalination, wastewater treatment, food and beverage processing, biotechnology, and petrochemical processing. Membrane-based separation processes are typically characterized by advantages such as selective separation, low space requirement, low chemical requirement, operational simplicity, and ease of process automation. Despite these advantages, permeate flux decline is one of the main limitations in membrane-based technologies. The flux decline is mainly attributed to the concentration polarization and membrane fouling phenomena. Membrane fouling is a complex phenomenon that involves deposition of materials on the membrane surface or within the membrane pores. Membrane fouling presents a greater challenge and contributes significantly to the decline in flux, productivity, and membrane lifespan, increase in the energy consumption due to high feed pressure requirement, and increase in the membrane maintenance, cleaning, and replacement costs. Therefore, research investigations into fouling control and membrane cleaning methods are of considerable importance.

Membrane cleaning methods are typically used when fouling control methods fail and the membrane must be cleaned for full or partial removal of the foulants. Cleaning methods may be classified into chemical or physical methods. Chemical cleaning methods involve application of chemical agents such as caustic soda, oxidants, acids, chelates, or proprietary surfactants in order to weaken cohesion forces between the foulants and the membrane surface. These methods usually require large amount of chemicals, pose safety concerns, cause damage to the membrane, and generate waste streams that can result in secondary pollution. Physical cleaning methods, on the other hand, involve application of hydraulic or mechanical cleaning forces in order to loosen and detach the foulants. Ultrasound application provides an alternative technique for membrane cleaning in desalination and water treatment. Critical analysis into the existing literature has been completed to establish the work plan. It is observed that although there are some experimental studies on the use of ultrasound in different membrane-based technologies, experiments at different scales of operation to understand the scale up issues are lacking. Also using pretreatment based on ultrasound and then investigating the membrane performance has not been studied extensively. The present project will deal with using ultrasound for membrane cleaning as well as in situ operation in the membrane processing. The effect of ultrasound on dyes in terms of degradation will also be studied as dyes give significant fouling effects on membrane especially in the wastewater treatment applications. The experimental configuration for membrane processing has been finalized. Nanofiltration polyamide flat sheet membrane of molecular weight cut off (MWCO) 100 to 250 D will be used.

Similarly for the dye degradation studies using ultrasound, initial experiments based on the effect of operating parameters have been completed. Reactive Yellow 135 (RY135) has been selected as the model compound for degradation studies using ultrasound. The effects of various operating parameters such as power, pH of solution, temperature, dye initial concentration and H2O2 dosage on the degradation rate were studied. The maximum degradation of RY135 was found to be 80.6% at the optimized conditions of power as 140W, pH of 2.5, temperature of 400C, initial concentration of 15ppm and dye to H2O2 ratio of 1:30 (v/v). Use of ultrasound has showed promising results for dye degradation. The work will be extended to combination with other oxidants as well as hydrodynamic cavitation for establishing the scale up prospects.

Research Student –Rutuja S. Bhoje

Project Title :	Graphene based Desalination membrane	
Supervisor from ICT:	Dr. P.R.Nemade, Department of Chemical Engineering Institute of chemical Technology, Mumbai	

After development of commercially successful m-phenylene diamine & 1,3,5-benzene tricarboxylic acid chloride or trimesoyl chloride (MPD &TMC) based thin film composite sea water reverse osmosis (SWRO) membranes, its performance enhancement in terms of productivity is always remain a thrust area of research. In this work, thin film composite (TFC) based SWRO membranes were prepared by interfacial polymerization of polyamide thin films over pure polysulfone (PSf) and polysulfone - graphene oxide nanocomposite (PSf-GO) support membranes. The nanocomposite support membranes were prepared with different concentration of GO varied from 0.25 – 1.0%. Subsequently TFC polyamide membranes were prepared over PSf and PSf-GO support membranes by in-situ interfacial polymerization using MPD in aqueous solution and TMC in isopar-G solvent. The TFC membranes were prepared using all different support and characterized in terms of product permeability and separation of NaCl solute under SWRO testing condition.

Flux and polyethylene oxide-100kDa rejection data is given in Fig. 1 and it is found that flux increases without change in single uncharged solute rejection. Higher water flux with similar rejection of uncharged solutes indicates that GO does not create any defect in the polysulfone membrane. Flux enhancement was also found in the SWRO membranes and it is more than twice in TFC membrane prepared from the support with optimized GO concentration as compared to the normal PSf support membrane (Fig.2). Graphene oxide makes polysulfone membrane more hydrophilic with rougher surface.

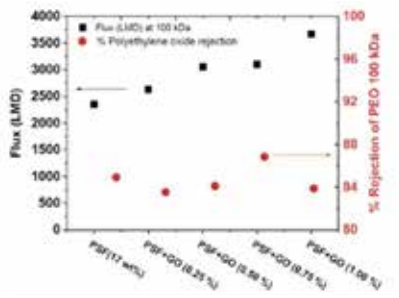


Fig. 1

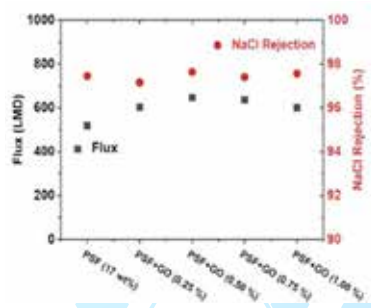


Fig. 2

Research Student : Satyajeet Shivraj Yadav

Project Title :	Development of hydrodynamic flow focusing droplet generator for preparation of mono- disperse actinide oxide microsphere	
Supervisor from ICT:	Prof. A. B. Pandit, Department of Chemical Engineering, Institute of chemical Technology, Mumbai	

In the advent of fast depleting non-renewable energy resources across the globe, nuclear energy is an important alternative source that needs to be utilized to its full potential. It is one of the cleanest forms of energy, as it does not generate greenhouse gases and leaves no residual effect on the environment. Oxides, carbides, nitrides and silicides of uranium, thorium and plutonium and their solid solutions have been used as nuclear fuels in various reactors. Most of nuclear reactors utilize fuel in the form of pellets that are stacked inside a metal cladding. The 'Sphere-Pac' fuel pin, an alternate form of fuel design has been developed to make the fuel fabrication process simpler and more amenable for remotisation. In the 'Sphere-Pac' fuel pin, fuel in the form of microspheres is packed into a metal cladding by the vibrocompaction process wherein mechanical vibrations aid in the process of packing. These processes have the advantage of being free from using radioactive powder and being suitable for adaptation to remote handling. They also have the potential to be used for the fabrication of fast reactor fuels as well as fuels containing minor actinides for the transmutation reactors.

In spite of the potential advantages of sphere-pac fuel, sol–gel based methods are yet to reach the realm of commercial fuel fabrication. This is due to the concerns regarding the fuel pins fabricated through vibrocompaction of sol–gel derived microspheres. The two major concerns are: (i) In the sphere-pac fuel pin, two or more size fractions of microspheres are needed to be vibrocompacted to achieve a smeared density of less than 80% of the theoretical density, ii) Microsphere for sphere-pac pin require to meet stringent quality control requirements with respect to dimensional tolerances and surface defects. Thus, there is need of single system capable of producing, two (or more) size fractions of microspheres with desired properties.

In the present work we are using hydrodynamic flow focusing droplet generator for preparation of monodisperse actinide oxide microspheres. Ammonium ceric nitrate which is non-radioactive surrogate of plutonium is used. Two different sizes of microspheres (2800 & 500 μm) are fabricated using a single prototype. Size measurement is done using Image J analysis software. The effects of the flow rate of the continuous and dispersed phase on the size and size distribution of Cerium microspheres were investigated. A comprehensive characterization of the Cerium microspheres has been conducted, including the X-ray diffraction pattern, EDX, FTIR, SEM, density, size, and size distribution. The size of the prepared monodisperse microspheres can be controlled precisely in the range of 100 to 3000 micrometers and the coefficient of variation of the size distribution is below $\pm$5%.

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Research Student: Bhujbal Akshay Vilas

Project Title:	Electrochemical behaviour of U (III), Al (III) and Zr (IV) in Ionic liquid medium	
Project Investigator:	Prof. Bhalchandra M. Bhanage, Department of Chemistry, ICT Mumbai 400019	
Co-Investigator:	Dr. K. A. Venkatesan, Indira Gandhi Centre for Atomic Research, Kalpakkam, Chennai.	

- Electrochemical behaviour of Uranyl ion is studied in ammonium ionic liquid by various transient electrochemical techniques such as cyclic voltammetry, Chronoamperometry and Chronopotentiometry.
- Novel process has been developed for the electrodeposition of Uranium dioxide nanoparticles from Uranyl Nitrate ammonium based ionic liquid
- Range of Novel Protic ionic liquids are synthesized and feasibility of dissolution of Aluminium chloride is studied for electrodeposition of aluminium.
- Currently, suitable ionic liquids for the further studies like electrodeposition of metallic Uranium is being explored
- Solubility of AlCl3 in various protic ionic liquids is also in progress.

Figure. 1: *Electrochemical gas tight cell developed in order to maintain inert atmosphere for the electrochemical study of aluminium*

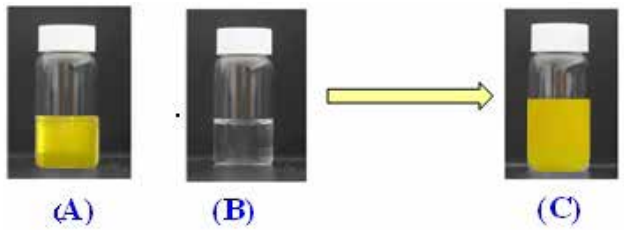
Conference Papers

Bhujbal, A.V.; Bhanage, B.M.; Rout, Alok; Venkatesan, K.A. Direct electrodeposition of UO2 from Uranyl nitrate dissolved in tri-n-butylmethylammonium chloride ionic liquid; Proceedings of the fourteenth biennial DAE-BRNS symposium on nuclear and radiochemistry; 15-19 Jan 2019.

Research Student: Esha Attar

Project Title:	Bioenhanced & Targeted Drug Delivery System of Deuterated Mitrocurcumin
Principal Investigator:	Prof. Padma V. Devarajan
Co-Investigator:	Prof. Mariam S. Degani, Institute of Chemical Technology, Mumbai

The project deals with the synthesis of Deuterated Mitocurcumin and development of bioenhanced lung targeted formulations of Mitocurcumin and Deuterated Mitocurcumin for delivery by a route of administration that is very patient friendly and acceptable namely the oral route.



Process of formation of solid lipid nanoparticles of curcumin

The availability of Mitocurcumin is limited. Hence solid lipid nanoparticles of Curcumin (as a surrogate for Mitocurcumin) are developed. They are optimized for size and entrapment efficiency and based on this study solid lipid nanoparticle of mitocurcumin were successfully prepared. As the next step we have incorporated the lung targeting ligand Gantrez (polymethyl vinyl maleic anhydride copolymer) and prepared Curcumin nanoparticles. We achieved desired average size of ~400 nm size with <0.3 polydispersity index and >80% entrapment efficiency. Incorporation of Gantrez was confirmed by FTIR and mucoadhesion monitored.

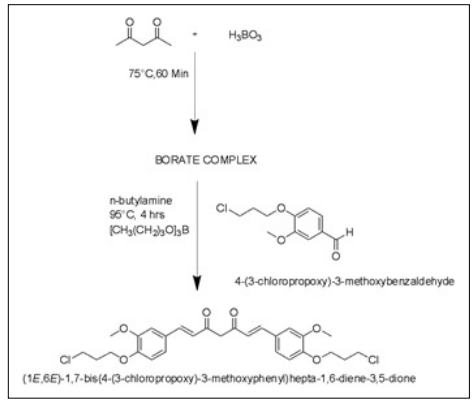
Solid lipid nanoparticles of Mitocurcumin formulated with similar strategy of curcumin which revealed no change in entrapment efficiency, however a marginal increase in size compared to curcumin nanoparticles was observed. Further a significant increase in size was observed at 2 hours suggestive of instability. Further work would involve optimizing the mucoadhesion and hydrophobicity and transferring the method to preparation of solid lipid nanoparticles of Mitocurcumin. In vitro efficacy in cancer cell lines and in vivo efficacy in preclinical model will be the next steps.

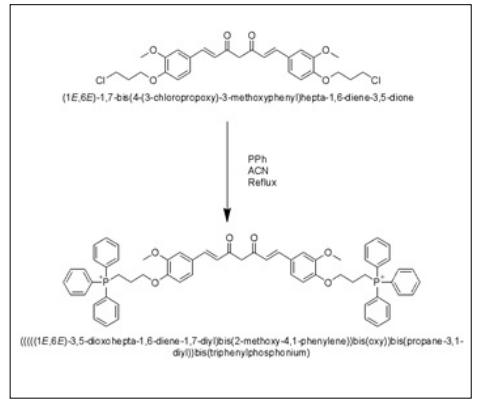
Research Student: Vishakha Likhite

Project Title:	Bioenhanced & Targeted Drug Delivery System of Deuterated Mitrocurcumin
Principal Investigator :	Prof. Padma V. Devarajan
Co-Investigator:	Prof. Mariam S. Degani, Department of Pharmaceutical Sciences and Technology Institute of Chemical Technology Mumbai

Synthesis and Characterization of Mitocurcumin

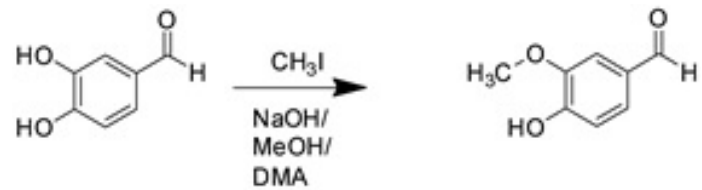
Curcumin is a major constituent present in an Indian herb Curcuma longa, and has been shown to possess many pharmacological properties including anti-infective & anticancer. Mito-curcumin (Derivative of curcumin) has been successfully synthesized from o-alkylated vanillin, using suitable modifications of reported procedure. (1)





Deuteration of Curcumin

As curcumin can be synthesized from vanillin, model reactions for synthesis of deuterated vanillin are being carried out.



In vitro anti-cancer efficacy

Vanillin and 'mitolated' vanillin are being tested against various anti-cancer cell lines.

Metabolic Studies

Isolation and estimation of protein content from rat liver microsomes for metabolic stability is carried out.

Reference

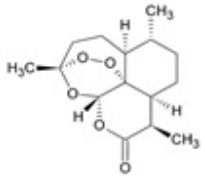
- Pabon HJ. A synthesis of curcumin and related compounds. Recueil des Travaux Chimiques des Pays-Bas. 1964;83(4):379-86.

Research Student: Kranti Kamble

Project Title:	Extraction and Deuteration of Natural Products of Therapeutic importance for Improved Potency
Principal Investigator:	Prof. K. S. Laddha
Co-Principal Investigator:	Dr. Shreerang Joshi
Principal Co-ordinator:	Dr.D.Goswami (BARC), Department of Pharmaceutical Sciences and technology, Institute of Chemical Technology, Mumbai

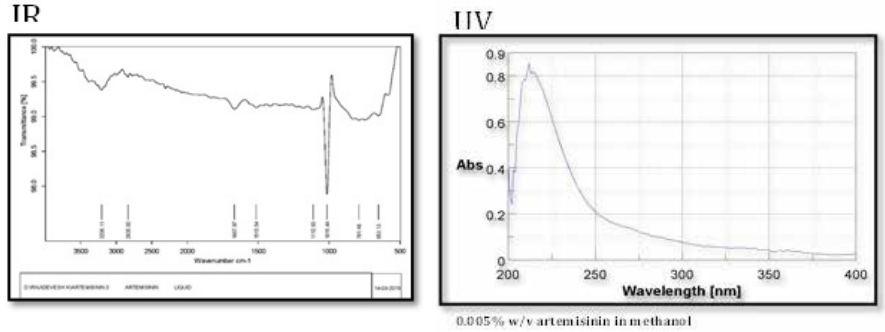
Artemisinin is a sesquiterpene with a tetracyclic structure with a trioxane ring and a lactone ring. The trioxane ring contains a peroxide bridge, the active moiety of the molecule. Artemisinin and its derivatives are renowned for their potent antimalarial activity.

Extraction and isolation of Artemisinin: Dry Artemisia leafy biomass treated with solvent (petroleum ether) artemisinin extraction (10 h.at 30-450C) to get raw extract containing solvent, artemisinin, wax, chlorophyll, essential oils, etc. Further extract with ether, ethyl acetate, water, air. Chromatographically isolate artemisinin, wash it with cold ether. Recrystallize artemisinin with 5% alcohol.



Artemisinin powder yield 2gm

Characterization of Artemisinin:



Research Student: Ashwani S. Patil

Project Title :	Modified deuterated polyphenols as chemotherapeutic and antimicrobial agents	
Principal Investigator:	Prof.Mariam S Degani, DPST, ICT	
Co-Principal Investigator:	Prof. Sadhana Sathaye, DPST, ICT	

Polyphenols are very well known to possess anti-cancer and anti-microbial activity. However, the main disadvantage of natural polyphenols is their poor bioavailability in both plasma and tissues.Thus, their conversion to 'mito'- polyphenols by linking totriphenylphosphine could enhance their activity and target it into mitochondria.

- Developed HPLC method for parent compounds and their mito derivatives such as Pterostilbene, Mito-Pterostilbene, Ethyl ferulate, Mito Ethyl ferulate, Vanillin, Mito-Vanillin, Apocynin and Mito-apocynin in a same mobile phase for parent and mito one for accuracy and convenience while doing metabolic stability assay.
- Rat liver microsomes (RLM) isolation for the metabolic stability study of these synthesized polyphenols.
- Protein content for the isolated Rat liver microsomes was performed.
- Procedure for the metabolic stability with rat liver microsomes was optimised after many attempts with standard drug Diclofenac to confirm the isolated microsomes are working.

- Metabolic stability for Pterostilbene has been done and found to be metabolically stable with rat liver microsomes, ethyl ferulate was found to get metabolised by RLM whereas for other compounds the work is in progress.
- Have started evaluation of anti-cancer activity at BARC of synthesised polyphenols, and also found the significant difference in the activities the mito derivatives as compared to the parent molecule.

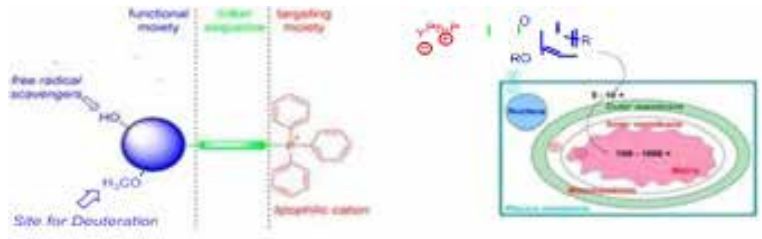
Research Student: Mahin K I

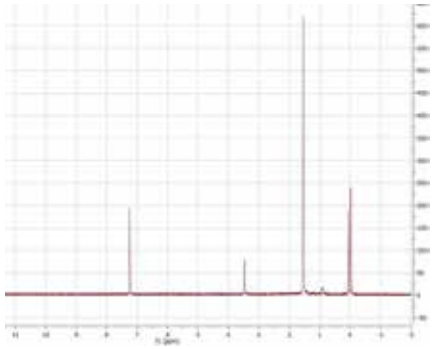
Project Title :	Modified deuterated polyphenols as chemotherapeutic and antimicrobial agents	
Principal Investigator:	Prof. Mariam S Degani, DPST, ICT	
Co-Principal Investigator:	Prof. Sadhana Sathaye, DPST, ICT	

Several natural polyphenols are known to have good anti-cancer and anti-microbial activity. However, the main disadvantage of natural polyphenols is their poor bioavailability in both plasma and tissues. Thus, their conversion to 'mito'- polyphenols by linking to triphenylphosphine could enhance their potency. Deuteration could further increase their potential half-life, thus making the molecules promising for further clinical testing. The project envisages improvement of activity and metabolic stability by mitolation and deuteration at strategic positions on polyphenols.

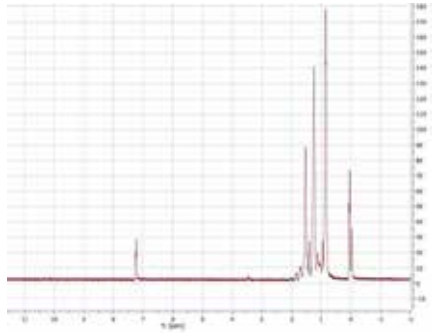
- We have synthesized four mito-polyphenols with a triphenylphosphine moiety attached via a suitable linker (Mito-Pterostilbene, Mito-Vanillin, Mito-Apocyanin and Mito-Ethyl Ferulate) and their structures have been characterised.

- Biological evaluation of these mito-compounds are ongoing. This includes metabolism studies as well as anticancer testing. Initial results for enhanced mitochondrial penetration are promising.
- Model reactions for deuteration have been initiate





General Structure of Mito-Polyphenol



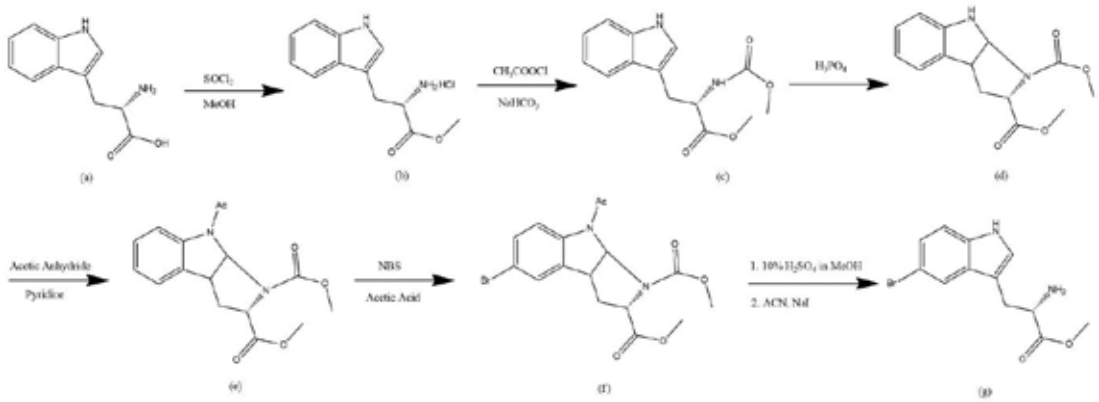
Cellular uptake of TPP+-linked compounds to mitochondria

Research Student: Sandeep R. Avadutha

Project Title:	Deuterated Amino Acids for Possible Increase of Lifetime of an Active Drug	
Research Supervisor:	Prof. S.V. Joshi, Dept. Pharmaceuticals Sciences and Technology Institute of Chemical Technology, Mumbai	

Deuterated Amino Acids finds an important application in today's world of drugs synthesis as it reduces the half life of an active drug by a significant amount and due to which it spends more time in the body and there is an increase in the lifetime of an active drug which results in the less dosage.

Synthesis of 5-Br-Tryptophan Methyl Ester(g)



At present compounds (d) and (e) are under preparation.

Compounds (b) and (c) have been successfully synthesized and characterized by melting point and recording FT-IR, NMR spectra respectively.

Conversion to (g) is the next target.

Reference: Garcia JM, Curzon SS, Watts KR, Konopelski JP. Total Synthesis of Nominal (11 S)-and (11 R)-Cyclocinamide A. Organic letters. 2012 Apr 5;14(8):2054-7.

Research Student: Sumeet Sangram Sonvane

Project Title:	High Performance Laser Dyes Design and Synthesis	
Research Supervisor:	Prof. N. Sekar, Institute of Chemical Technology, Mumbai	

Experimental Setup: Synthesis of dye

Organic dyes with delocalized □-electrons have been used invariably as gain medium in laser dyes. Thus the perennial problems in colorants used in dye lasers remain good (~1 mM) solubility in ethanol, methanol, and water solvents, good absorption cross sections at available wavelengths of visible pump lasers, high quantum yield of fluorescence and high photochemical stability under laser operation. Improvement in photochemical stabilities as well as quantum yield of fluorescence of new organic dye molecules at intended wavelengths is a subject of high interest for research. In this study, we have synthesized modified BODIPY dye for laser study. In this dye chemically active fluorine atom at boron centre reduce its photostability and quantum yield of fluorescence. To overcome this problems, we have replace -F atom by –CN group which shows enhanced quantum yield of fluorescence. We have calculated fluorescence quantum yield of the cyano BODIPY comparing with fluoro BODIPY. Computational studies of the BODIPY dyes were done by using DFT/TD-DFT method. Cyano BODIPY shows better charge transfer characteristics and good stability than fluoro BODIPY. The aim of this study is enhancement of the quantum yield of fluorescence and laser efficiency.

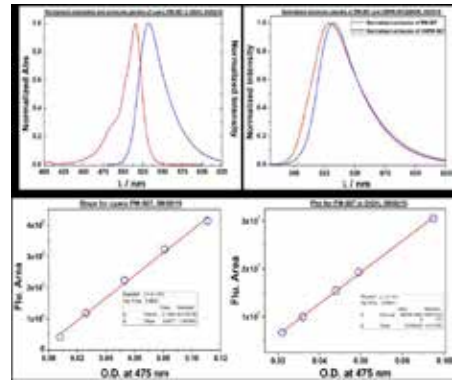


Figure: Photophysical study of Cyano BODIPY

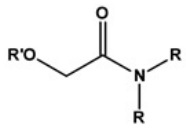
Quantum yield of Fluorescence (□) of Cyano BODIPY = 0.93 in ethanol solvent.

Research Student: Amid Laxman Sadgar

Project Title:	Synthesis of N,N-dialkyl-2-alkoxyacetamides extractants and N,N-dialkyl-2- alkoxyacetamide grafted resins for the separation of trivalent actinides from nitric acid medium and modeling of extractants	
Research Supervisor:	Prof. R.V.Jayaram, Institute of Chemical Technology, Mumbai	

The aqueous product (PUREX raffinate) discarded after the separation of uranium and plutonium during the reprocessing of spent nuclear fuel known as "high-active waste" (HAW). Which is a complex mixture of several alpha-emitters such as 241Am, 243Cm and 239Np (known as minor actinides), fission products, corrosion products of structural materials and the additives etc. Among the radionuclides present in HAW, minor actinides contribute to maximum radiotoxicity. The long term concerns of the waste can be minimised and eliminated by a partitioning and transmutation strategy. It involves the separation of Am(III) from HLLW and transmute the same in to stable or short lived radionuclides in the advanced fast reactor.

The current method for actinide separation involves solvent extraction of trivalent actinides and coexisting lanthanides from HLLW using suitable solvents. Among the various reagents reported for the extraction of trivalent actinides from nitric acid medium, diglycolamides have received considerable attention in the past few decades. The DGA's are N,N,N'N'-tetraalkyl-3-oxypentane 1,5 diamide derivatives which act as tridentate ligands. However they have limitations like third phase formation, extraction of unwanted metal ions etc. It was realised that the presence of etheral oxygen at the 2-position in DGA makes these reagents superior to other amide base extractants. It is likely that the etheric functional moieties as in N,N-dialkyl-2-oxyacetamides would be sufficient for extraction of Am(III). Since the other amidic functionality is not available in such 2-oxyacetamide derivatives, it is expected that these reagents would not extract the unwanted metal ions. Hence, the project aims to synthesize N,N-dialkyl-2-oxyacetamides (Alkyl=C6,C8,C10,C12,sym metrical and unsymmetrical) and 2-oxy N,N-dialkyl acetamide grafted resins for the extraction of Am(III) and Eu(III) from nitric acid medium.



$R = C_6H_{13}, C_8H_{17}, C_{10}H_{21}$

$R' = C_6H_{13}, C_8H_{17}, C_{10}H_{21}$

Structure of amides

Publications:

No.	Authors	Title	Journal	Vol. No.	Pages	Year
1	S. N. Gosavi, N. J. Kulkarni, C. S. Mathpati, D. Mandal	CFD modeling to determine the minimum fluidization velocity of particles in gas-solid fluidized bed at different temperatures	Powder Technology	327, 2018	109-119,	2018
2	Farakte, R.A., Hendre, N.V. and Patwardhan, A.W.	CFD Simulations of Two Phase Flow in Asymmetric Rotary Agitated Columns	Industrial & Engineering Chemistry Research	57(50)	17192-17208	2018
3	Urunkar, Y.; Pandit, A.; Bhargava, P.; Joshi, J.; Mathpati, C.; Vasanthakumaran, S.; Jain, D.; Husain, Z.; Patel, S.; More, V.	Light-Weight Thermal Insulating Fly Ash Cenosphere Ceramics	International Journal of Applied Ceramic Technology	15 (6)	1467–1477. DOI: 10.1111/ijac.12906	2018
4	Hendre, N.V., Venkatasubramani, V., Farakte, R.A. and Patwardhan, A.W.	Hydrodynamics and mass transfer characteristics of asymmetric rotary agitated columns	Industrial & Engineering Chemistry Research			2018
5	Shashank S. Tiwari, Shivkumar Bale, Ashwin W. Patwardhan, Krishnaswamy Nandakumar and Jyeshtharaj B. Joshi	Insights into the physics of dominating frequency modes for flow past a stationary sphere: Direct numerical simulations	Physics of Fluids	045108		2019
6	Shashank S. Tiwari, Eshita Pal, Nitin Minocha, Shivkumar Bale, Ashwin W. Patwardhan, Krishnaswamy Nandakumar and Jyeshtharaj B. Joshi	Flow past a single stationary sphere, 2. Regime mapping and effect of external disturbances	In Press, Powder Technology			2019
7	Shashank S. Tiwari, Eshita Pal, Nitin Minocha, Shivkumar Bale, Ashwin W. Patwardhan, Krishnaswamy Nandakumar and Jyeshtharaj B. Joshi	Flow past a single stationary sphere, 1. Experimental and Numerical Techniques	In Press, Powder Technology			2019
8	Gaikwad G, Jain R and Dandekar P	Microdevice for Nanoparticle and chemical Synthesis	The Patent Office Journal	18(3)	19357	2019
9	Gaikwad G, Jain R and Dandekar P	Microreact or platform for Nanoparticles synthesis	The Patent Office Journal	28(4)	30501	2019
10	Gaikwad G, Gore M, Jain R and Dandekar P	Biomimetic Gut Multi-Well Plate	The Patent Office Journal	23(3)	24708	2019
11	Sawant, S.V., Banerjee, S., Patwardhan, A.W., Joshi, J.B. and Dasgupta, K.	Effect of in-situ boron doping on hydrogen adsorption properties of carbon nanotubes	International Journal of Hydrogen Energy		2019	
12	Sabnis, Sarvesh S. & Gogate, Parag R.	Ultrasound Assisted Size Reduction of DADPS Based on Recrystallization	Ultrasonics Sonochemistry	54. 10.1016/j.ultsonch. 2019. 01. 037		2019
13	Zakir Husain, Khursheed B. Ansari, Vikram S. Chatake, Yogesh Urunkar, Aniruddha B. Pandit & Jyeshtharaj B. Joshi	Valorisation of biomass pellets to renewable fuel and chemicals using pyrolysis: characterisation of pyrolysis products and its application	Indian Chemical Engineer, Taylor & Francis	DOI: 10.1080/00194506.2019.1635047		2019