# 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

| Sr. No. | 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 |

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|---|---|---|---|---|
| 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 |

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

| Sr. No. | Name | Title of Ph.D. Project | Previous Institute | Qualification | Supervisor |
|---|---|---|---|---|---|
| 1. | Vishal Sawant | Design and synthesis of extractant for selective extraction of metal ions from nuclear Waste | Mumbai University | M.Sc. | Prof. V.G. Gaikar |

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| 2. | Bhavesh Gajbhiye | Thermal hydraulic studies related to coolants for new generation reactants | ICT, Mumbai | M. Chem. Eng | Dr. C. S. Mathpati |
| 3. | 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 |
| 4. | Zakir Hussain | Modelling and simulation of solid fuel burning devices | UDCT, Jalgaon | M. Tech. | Prof. A. B. Pandit |
| 5. | Swapnil Chaudhari | Transport of actinides and fission products across hollow fibre supported liquid membranes | ICT, Mumbai | M.Tech | Prof. A. V. Patwardhan |
| 6. | Anita Sharma | Synthesis of carbon nanotubes | ICT, Mumbai | M. Tech. | Prof. A. W. Patwardhan |
| 7. | Rajput Swapnil K | Development of grafted resins and membranes (extractants) for precious metals | ICT, Mumbai | M.Chem.engg. | Prof. Anand V. Patwardhan |
| 8. | Tiwari Shashank S. | Transport Phenomenon in Gas- Solid Systems | NIT, Bhopal | M.Tech. | Prof. A.W Patwardhan. |
| 9. | Gaikwad Ganesh | Conjugation and radiolabeling of various nanoplatforms for image guided theranostic applications | UDCT, Jalgaon | M.Tech. | Prof. V.G. Gaikar |
| 10. | Hendre Nilesh V. | CFD Modeling of Asymmetric Rotating Disc Contactors | NIT, Trichy | M.Tech. | Prof. A. V. Patwardhan |
| 11. | Shruti Hinge | Computational fluid dynamics of the stirred reactors | ICT, Mumbai | M.Chem. Engg | Prof.A.W. Patwardhan |
| 12. | Pratiksha Madhukar Biranje | Synthesis and modification of carbon nanotubes modelling experimentation and applications | ICT, Mumbai | M.Tech. (Oils) | Prof.A.W. Patwardhan |
| 13. | Amol Vilas Ganjare | Development of grafted membranes (extractants) for radioactive and other metals. | ICT, Mumbai | M.Tech (Oils) | Prof.A.V. Patwardhan |

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| 14. | Shrilekha Vijaysinh Sawant | Synthesis and modification of Carbon nanotubes: Modeling, Experimentation and Applications | ICT, Mumbai | M.Tech. Green Technology | Prof.J.B. Joshi |
| 15. | Tukaram Udhavrao Shinde | Mathematical modelin of the Gas centrifugal separator | LIT Nagpur | M.Tech. | Dr. V.H. Dalvi |
| 16. | Sarvesh Sanjay Sabnis | Improved Separations and Cleaning Using Ultrasound | ICT Mumbai | M.Tech. | Dr. Parag R. Gogate |

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

| Sr. No. | 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. | PravinBote | Novel reactor design for synthesis of different oleochemicals | Prof. V.G. Gaikar |

## DAE ICT CENTRE FOR CHEMICAL ENGINEERING EDUCATION AND RESEARCH

Shruti Hinge

**Project** : Computational fluid dynamics of the stirred reactors
**Supervisor from ICT** : Prof. Ashwin Patwardhan

Stirred reactors are the most widely used reactors to carry out different type of reactions. These reactors can be operated in batch, semi batch or continuous mode. There is a wide distribution of velocity, kinetic energy, temperature, concentrations etc. inside the reactor. Big fluctuations in these parameters can have adverse impacts on yields and also on the quality of the product. CFD can be a useful tool to design such reactors and improve its performance using mathematical and computational modeling method.

**Summary of the Work Done:**

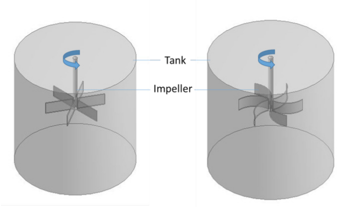
1. Study of the basics of computational fluid dynamics
2. Study of the theory related to the stirred reactors
3. Use of ANSYS FLUENT for geometry creation, mesh generation
4. Literature survey related to various stirred reactors, which summarize the following about the work carried out by previous authors:

- type and size of reactor
- batch/semi batch/ continuous
- type of impeller
- baffled/un-baffled

- turbulence model
- two phase model
- how the impeller is modeled
- phases considered
- number and shape of grids
- if heat transfer is considered
- if liquid rheology is considered
- if time dependency is considered
- experimental validation
- 2-D/3-D modeling
- CFD software packages used

**Proposed Work:**

1. In depth literature survey and concluding remarks
2. Case study to reproduce the work by previous authors
3. CFD of a system with known parameters
4. Experimental validation of the results

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## Pratiksha Madhukar Biranje

**Project** : Synthesis and modification of carbon nanotubes: modeling, experimentation and applications

**Supervisor from ICT** : Prof. Ashwin Patwardhan

**Co-Investigator** : Dr. J. B. Joshi

Carbon nanotubes (CNTs) are promising candidates for a wide range of applications that are expected to improve our life-styles, such as alternative forms of energy production, energy storage, and drug delivery. At the same time, there are concerns about their possible adverse effects on human health, since there is evidence that exposure to CNTs induces toxic effects in experimental models. However, CNTs are not a single substance but a growing family of different materials possibly eliciting different biological responses. As a consequence, the hazards associated with the exposure of humans to the different forms of CNTs may be different. Understanding the structure–toxicity relationships would help towards the assessment of the risk related to these materials. Here, we present a snapshot of the current state-of-the art of CNT production, applications, and safety.

**Work Done:**

1. Understanding the topic details
2. Reviewing the plan of action

**Future Work:**

1. Complete the literature survey regarding topic
2. Understanding the gaps and holes in the theory
3. Designing the experiments
4. Start experimental work

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## Amol Vilas Ganjare

**Project** : Development of grafted membranes (extractants) for radioactive and other metals.

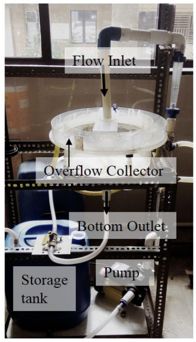
**Supervisor from ICT** : Prof. A.V. Patwardhan

Solvent extraction is widely used for the purification and concetration of metals and recovery of spent nuclear fuels. Solvent extraction traditionally performed in mixer-settlers, batch vessels, extraction columns or centrifugal extractors. In the traditional operations the feed liquid is dispersed into the extraction solvent. Various problems like formation of a stable emulsion, foaming or flooding are encountered in above discussed methods. An improved extraction can be achieved by membrane separation. In membrane separation, the liquids flow along both sides of this membrane.The pores of the membrane are filled with the liquid and the interface is pinned by capillary action. The extraction degree of compound depends on the composition of initial and final solutions. The extractant act as a transporter and interact with the extracted substance during its transport from initial into the final phase.

Separation with membrane shows a superior preconcentration effect and cleaning capability for trace metals and radionuclides. It also allow to use expensive but selective and resistant extraction reagents efficiently. Kinetic effects can be used for specific separation. The main points of inconvienice are breakdown of membranes, transport of acids, and formation of surface active radiolysis products in case of radioactive metals.The effective grafting of membrane for effective extraction and for dealing with the discussed inconviences in the membrane process are the main focus of current work.

**Highlights of the Work Done:** Literature survey for the work done in the field of extraction for the heavy metal and the same with the use of membranes and the grafted membranes is done in last three months. This will help to select and manage the system parameters for the extraction of radioactive and other metals with the help of membranes.

**Proposed Work:** Design of the system for the extraction is to be done in near future. The process of grafting of membrane will be studied. Literature will be done for the selection of grafting material and the method.Once the grafting parameters are set membrane grafting and the separation will be carried out.




Experimental Setup: Secondary Settling Tank

Shrilekha Vijaysinh Sawant

**Project** : Synthesis and modification of Carbon nanotubes: Modeling, Experimentation and Applications

**Supervisor from ICT** : Prof. Ashwin patwardhan

**Co-Investigator** : Prof. J.B. Joshi

A carbon nanotube (CNT) is a tube shaped material, made up of carbon, having a diameter measuring on the nanometer scale. These structures have an array of fascinating electronic, magnetic and mechanical properties. CNTs have high tensile strength approximately 150GPa, which is 100 times more than stainless steel. They have high modulus (1 TPa) and large aspect ratio. All these properties and their applications in different fields increased the interest in CNTs. In the present work, we are mainly focusing on synthesis of carbon nanotubes. Synthesis in different reactors affects the shapes and sizes of CNTs.

**Highlights of the work done in 2016-17:**

1. Experiments are designed for synthesis of single walled-multi walled CNTs.
2. Literature study for synthesis of Boron-doped carbon nanotubes.

**Comments:**

Single walled- multi walled carbon nanotubes can be synthesized by mainly chemical vapor deposition (CVD) and varying carbon precursor, catalyst and substrate. Supply of carbon reactant is important to the growth of large diameter nanotubes. Similarly, for achieving high-quality large diameter nanotubes, growth temperature is important. Appropriate selection of CNTs precursor and reaction conditions can increase the lifetime of catalysts, CNT-growth rate, quality and yield, e.g. ethanol as a precursor makes CNTs free of amorphous carbon due to etching of hydroxyl radicals.

B-Doped CNTs can be synthesized by CVD, using boric acid ($H_3BO_3$), trimethyl borate $B(OCH_3)_3$, $BF_3$, diborane ($B_2H_6$) as precursor. Boron atoms in CNTs acts as electron acceptors producing p-type CNTs. Therefore for characterization, Field emission spectroscopy and Raman spectroscopy are highly used.

**Proposed work in 2017:**

1. Synthesis and characterization of single walled- multi walled CNTs.
2. Synthesis of B-doped CNTs in fixed bed and fluidized bed reactors, and their kinetics.

Tukaram Udhavrao Shinde

**Project** : Mathematical modeling of the gas centrifugal separator
**Supervisor from ICT** : Prof. Ashwin Patwardhan
**Co-Investigator** : Dr. V. H. Dalvi

**Introduction:-**

The project aim is to mathematical model gas centrifugal separator and determine the order of magnitude of the maximum achievable separation for gas using a gas centrifugal separator.

**Highlights of the Work Done in 2016:**

1. Learning and understanding of fluid dynamics and heat transfer in Ansys and OpenFoam CFD software for various geometry and cases.
2. Literature survey of gas centrifugal separator for various problems related to the mathematical modelling.
3. A sample case study conducted a two dimensional computational simulation of closed room with heater. The typical closed house dimensions have been taken as reference for a closed room with a hot-pot placed in the middle of the floor. The physical model for present study is that of a heater having temperature of 580C placed in the center of room. Simulations show that while the heater loses heat at a sustainable rate, the temperature distribution is sub-optimal: with most of the warm zone being above the height of the floor. Hence a purely passive system could not be made to work effectively and a way to counter the natural convection currents is essential.

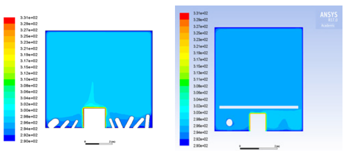
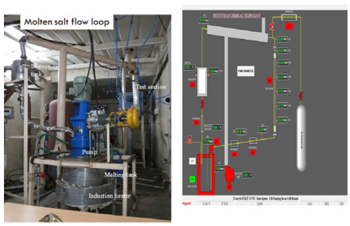


**Figure: Different geometry CFD simulation of heater placed in closed room for a study of natural convection heat transfer**

**Proposed Work in 2016-17.**

1. CFD study of 3D Gas centrifugal separator.
2. Solving mathematics of gas redefine regime in gas centrifugal separator.
3. Computational Study of applications of gas centrifugal separator for various gas separation industries.

**Experimental Set-up**



## Vishal Sawant

**Project** : Desgin and Process intensification of Novel Extractants for Selective separation of Metal Ions

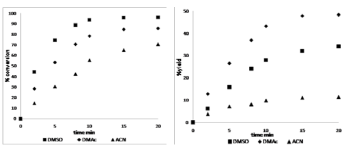
**Supervisor from ICT :** Prof. V. G. Gaikar

Microwave-assisted organic synthesis is a division of green chemistry, which has gained more attention in recent years. Microwave-assisted processes are pollution free, eco-friendly in nature. Microwaves transfer energy in 10-9 s with each cycle of the electromagnetic wave which is much faster than the kinetic molecular relaxation time 10-5 s. This results in non-equilibrium condition which leads to generation of the instantaneous high temperature. It was discovered that microwave irradiation offered, major improvements over conventional heating methods, including increased yields, shorter reaction times, cleaner reaction profiles, and improved selectivity.

The synthesis of crown ether compounds has been an extremely challenging process, especially to determine the most favourable synthetic routes.A rapid and convenient process for the preparation of dibenzo-18-crown-6 ether was developed. The reaction was carried out in a batch glass reactor under microwave heating. The influence of parameters, such as reaction time, solvent, base, and power of microwave irradiation on the reaction were studied.

The dibenzo-18-crown-6 ether was obtained with a moderate yield, along with shortened reaction time from several hours to several minutes as compared to the conventional heating method. The maximumpercentage yield of dibenzo-18-crown-6 ether was obtained to be 48.27% in the presence of the N, N-dimethylacetamide solvent at 900 W of microwave irradiation

**Results:**




A B

Figure 1: Effect of the reaction time on (A) % conversion of catechol and (B) %yield of dibenzo-18-crown-6 ether in the presence of potassium hydroxide and different solvents at 900 W of microwave irradiation.

**Experimental Unit** - Microwave Assisted Batch Reactor

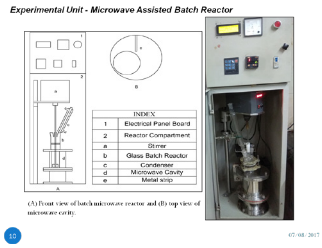



Figure 2: (A) Front view of batch microwave reactor and (B) top view of microwave cavity used in synthesis of dibenzo-18-Crown-6 ether

## Swapnil Rajput

**Project** : Project Development of grafted resins and membranes (extractants) for precious metals

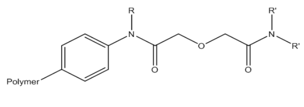
**Supervisor from ICT :** Prof. Anand V. Patwardhan

**Summary:**
The project aims to investigate novel separation approaches for recovery of radioactive elements from radioactive waste streams. The radioactive elements can be actinides such as U, Am (Eu can be used as a surrogate for studies carried out at ICT), and Sr, at concentrations relevant in the dilute radioactive wastes such as those emanating from quality control operations or radioactive laboratories. Traditionally, adsorption and precipitation are

used for removal of toxic metal ions from industrial effluents. This project would investigate the application of adsorptive as well as membrane-based separation involving resins coated with an organic extractant or grafted resins, which are surface modified by a chemical reaction to include active complexationsites. The aspects to be studied are: synthesis of various resins and various grafted polymers with suitable active sites; adsorption of metal ion accompanied by mass transport phenomena from liquid phase to solid surface; the accompanying physical/chemical interactions; and selectivity of extractant / resins at molecular level. Appending functional groups onto magnetic particles will be taken up.

**Workdone during 2016-2017:**
Different polymeric membranes of polystyrene and Polysulphone were synthesized. Synthesized diglycolamide derivatives were incorporated in membrane matrix to physically bound diglycolamide functionalities over polymeric support for actinide separation. Different plasticizers were tried to make the membrane more robust.

Merrifield resin has been chosen as polymeric support for synthesizing grafted resins with diglycolamide functionalities. Different combinations of spacer lengths were tried like butyl, hexyl and octyl on primary and secondary positions, to check which serves the purpose best for actinide separation from waste stream. A five step reaction scheme were followed for each synthesis. Operating parameters were optimized to give best results. 75 to 80% grafting was done, which was checked on CHNS. (**R** = Butyl, Hexyl and Octyl ;**R'** = Butyl, Hexyl and Octyl)



Diglycolamide grafted Merrifield Resin

## Sarvesh Sanjay Sabnis

**Project** : Improved Separations and Cleaning Using Ultrasound

**Supervisor from ICT :** Dr. Parag R. Gogate

Ultrasound (20 kHz to 1MHz) is widely used for intensification of different chemical and physical processing applications as it creates alternating low-pressure and high-pressure waves in liquids, driving the formation, growth and violent collapse of bubbles in the liquid which is described as cavitation. Cavitation causes the generation of high speed impinging liquid jets and strong hydrodynamic shear-forces as well as can induce chemical changes in terms of free radicals and local hot spots. These effects can be quite effective for crystallization, emulsification, deagglomeration, extraction, cell disruption, cleaning of surfaces etc. Ultrasonic cleaning is driven by the principle of energy release from the collapse of microscopic cavities near the dirty surface that can generate liquid circulation and turbulence (physical effects) detaching the fouling or dirt attached to the targeted surface. In addition, the physical effects can also lead to improved separations based on the elimination of the mass transfer resistances.

The present project will aim at detailed study for the two specific applications of cleaning (fouled membranes and metal surfaces) and improved separations. There is a drawback in using biocides or chemical cleaning agents because they tend to disrupt membrane pores or lead to corrosion in metals. So, ultrasound can be used as an alternative or as a supplementary measure to control fouling in membranes and for cleaning metal surfaces. In desalination, during the recovery of fresh water from saline water, a major operational problem is scale depositsthatreduce the separation efficiency. Thus it is important to remove the sparingly soluble scale forming components such as $CaSO_4$and $CaCO_3$. Use of ultrasound will be investigated for improved crystallization and separation of these components under conditions suitable for thermal desalination operations. Ultrasound can influence the initiation of crystal nucleation, can control the rate of crystal growth, ensuring that small and even-sized crystals are formed, leading to better removal of particles.

This will be first tested on a laboratory scale to prove feasibility and establish the required optimum parameters. Subsequently, the process will be transferred to a pilot (bench) scale and if found suitable, also to commercial level. In a lab scale study, it is important to optimize parameters such as frequency, power dissipation and geometry of reactor. The present project will aim at such detailed study for the two specific applications of cleaning and improved separations.

Fig 1. Ultrasound assisted crystallization

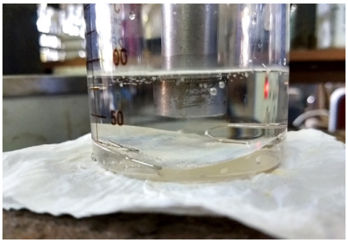


Fig 2: Sonication of fouled membranes.

**Summary of the work carried out during 2016-17:**

1. A detailed literature survey on ultrasound and its role in cleaning of fouled membranes, scaling management in membrane processes, cleaning effects of ultrasound on metal surfaces, sonocrystalization, etc. has been completed. The project objectives have been formulated based on the analysis of the literature
2. Initial strategy development for crystallization of CaSO4 to minimize seeding into the brine concentrator was devised.
3. Preliminary experiments regarding conventional (evaporative and cooling) crystallization and ultrasound assisted crystallization of saturated brine solution and its evaluation are completed.
4. Preliminary studies for understanding the effect of ultrasound generated using horn and bath on both normal and fouled membranes have been completed demonstrating the effects on morphology of membrane and extent of cleaning
5. Investigation of ultrasound on membranes with modified parameters so as to protect the membranes at the same time giving cleaning effect.

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Bhavesh D. Gajbhiye

**Project** : Thermal hydraulic studies related to coolants for new generation reactors

**Supervisor from ICT :** Dr. C. S. Mathpati

High temperature corrosion studies (650°C) in eutectic molten salt (FLiNaK) were carried out using salt purification and corrosion resistant coatings on different alloys. In this work, initial moisture content of eutectic mixture of FLiNaK salt was estimated by the Karl-Fischer titration method. Moisture removal was carried out by preheating and the vacuum drying method and subsequent corrosion studies were performed under inert nitrogen atmosphere. Effect of

Ni coating with different phosphorus content on corrosion characteristics for different alloys has been studied. Currently work on the hydraulics part of the project is in progress. Head loss coefficient due to different pipe fittings such as Tee, Bend, Elbow, Reducer etc. has been calculated using CFD in Ansys Fluent for different Reynolds number using water as fluid. Experiments have been planned to study the effect of flow assisted corrosion due to these different pipe fittings. Set-up has been fabricated and trial experiments have been done.

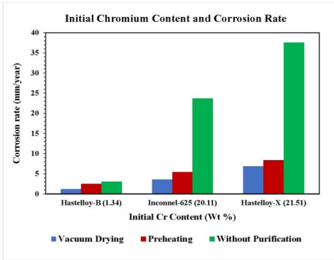


Figure 2: Correlation between corrosion rate and initial Chromium content

Figure1: Corrosion rate in molten salt with respect to Cr content in Alloy

**Equipments Purchased :**

1. 2 Crompton Greaves 0.5 HP Centrifugal Pumps – Rs. 5000.
2. Pipe fittings- Rs. 1000.

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## Sandeep Namdeo Gosavi

**Project** : 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

CFD modeling of unary gas solid fluidized bed in commercial software is being done and the results are being compared with experimental data. CFD simulations were done to study the effect of temperature on the minimum fluidization velocity. A research article is under review in Powder Technology. This has enabled to understand the basic modeling approach for GS fluidized bed and now we are moving to more complex scenarios. We are now studying the CFD simulations for effective thermal conductivity of packed bed.

1. Simulations of fluidized bed of Lithium Titanate at higher temperatures to ascertain the effect of temperature on minimum fluidization velocity were done.
2. CFD modelling of heat transfer of through packed bed with external heating was done.
3. ANN modelling to predict the effective thermal conductivity was done using the data from literature.A Matlab code was developed to get the coordinates of randomly packed spheres in a cylinder.
4. Code for finding the average coordination number of the packed bed was developed. It will be further used in developing code for heat transfer through the packed bed.
5. Geometry and Mesh was developed from this data. The mesh is currently under grid independency testing and improvisation.
6. The mesh generated using above code was successfully employed in the simulations of External Loop Air Lift Reactor with Packed Bed (ELALR-PB) in downcomer.

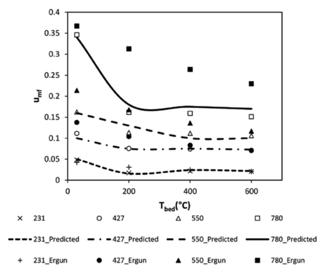



Figure 1: Minimum Fluidization Velocity at Different Temperatures (30, 200, 400 and 600 °C) for Different particle Sizes (231, 427.5, 550 and 780 µm)

**Conference Attended**

**S. Gosavi**, N. Kulkarni, C.S. Mathpati, D. Mandal, **Computational Fluid Dynamics of Heat Transfer**

**in packed bed and packed fluidized bed**, presented at 6th International and 43rd National Conference on Fluid Mechanics and Fluid Power (FMFP – 2016), December 15 – 17, 2016, MNNIT, Allahabad (India)

Zakir Husain Mohammed Yusuf

**Project** : Modeling and simulation of solid fuel burning devices

**Supervisor from ICT :** Prof. V. G. Gaikar

This part of study focuses on the use of Computational Fluid Dynamics to assist in the optimization of stove designs, with a hope to obtain a more concurrent strategy to obtain possible solutions to the problem of indoor air pollution and low efficiency of cook stove. Furthermore the study homes in on the CFD development of Eco biomass cook stove (EBCS) which is procured from Sanjay Technoplast Aurangabad, Maharashtra as shown in figure1a and figure1b. The stove is constructed from stainless steel. CFD modeling for the hydrodynamic studies of Eco biomass cook stove (EBCS) has been carried out in this part. Before studying the details of homogeneous and heterogeneous study in cook stove, it is essential to know the hydrodynamic study of cook stove. In the present work, a parameter study of biomass cook stove has been carried out for different flow rate of air. The effects of velocity of air, grate, orifice, and particles packed bed on the flow dynamics have been studied.

ANSYS 17.0 and Fluent used for Computational Fluid Dynamic simulations and analysis. ANSYS design Modular is used as a pre-processor to define the geometry (shown in figure2) of the model and to create a computational mesh. Fluent used to define boundary conditions for the problem (e.g. walls, velocity inlets for air and wood volatiles, pressure outlet etc.). Fluent solves the CFD model generated after various initial parameters are set. Fluent used as a post-processor to visualize and analyze the fluid flow. Color vector and contour plots may be created for parameters such as velocity, and pressure to assist in giving a visual representation of the fluid.

**Objectives**

The objective of this study is to ascertain feasiblemethods of applying technology that exists in the modern developed world to assist in solving the problem of indoor air pollution and low efficiency of cook stove. Furthermore to produce conclusive evidence that CFD can be used in a viable manner to assist in the development of smokeless cook stoves with higher heating efficiency.

To study the hydrodynamic study in EBCS we started with simple geometry i.e. empty eco biomass cook stove same as earlier case of hydrodynamics study.

Following configured geometry has selected for simplicity of work

To avoid complexity in the work we started with simple case1 i.e. empty eco biomass cook stove.

1. Empty Eco Biomass Cook Stove
2. Eco Biomass Cook Stove with grate at the bottom
3. Eco Biomass Cook Stove with orifice in the annulus space
4. Eco Biomass Cook Stove with grate at the bottom and orifice in the annulus space
5. Eco Biomass Cook Stove with grate at the bottom, orifice in the annulus space and particles

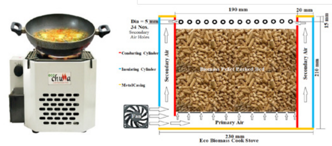


Fig1. (a) EBCS (actual model) Fig.1(b) Geometry of EBCS

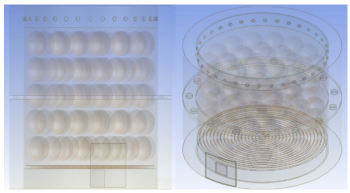


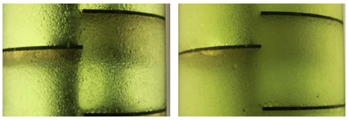
Figure2 EBCS with Grate at the bottom, Orifice in annulus space and Particles

## Mr. Nilesh Hendre

**Project** : Computational Fluid Dynamics Modeling of Asymmetric Rotating Disc Contactors

**Supervisor from ICT :** Prof. V.G. Gaikar

Hydrodynamics and mass transfer performance of asymmetric rotating disc column (ARDC) and asymmetric rotating impeller column (ARIC) have been carried out. Industrially, ARIC is used for the separation of uranium from wet phosphoric acid using an organo-phosphorous solvent. The two above mentioned columns, ARIC and ARDC are geometrically similar, except the type of agitator, used for dispersion of one phase into another. In ARIC, pitched blade-disc (PBD) impeller are used, whereas in ARDC, discs are employed for inducing agitation. The hydrodynamics characteristics of ARIC and ARDC have been studied at various operating conditions in a lab scale column (I.D.= 0.1 m, number of stages =15). Effect of two different liquid-liquid systems of different physical properties on the hydrodynamics characteristics such as drop size and hold up and axial mixing has been explored. With increase in agitation, decrease in drop size and increase in holdup of dispersed phase is observed. Mass transfer performance of ARIC for the extraction of uranium from phosphoric acid has been investigated at different agitation conditions. The percentage extraction of uranium has been found to increase from 36% at 150 rpm to almost 99% at 250 rpm.



500 rpm 800 rpm

**Equipment purchased:** ARIC (4" I.D.), Cost = 1,25,000/-

## Shashank Surendra Tiwari

**Project** : Direct Numerical Simulation of Flow Patterns in Multiparticle Systems

**Supervisor from ICT :** Prof. Ashwin Patwardhan

Multiparticle flows are encountered in a number of naturally occurring phenomenon as well as in artificially designed equipment. A large number of parameters such as the terminal settling velocity of the particles, drag, lift and other interfacial forces, void fraction depend on the separation angle at breaking of the axisymmetric wake in the downstream region of the particle which in turn depends on the hindrance effect due to neighbouring particles and also due to presence of wall. The adverse pressure gradient at the boundary layer causes it to transition from a laminar to turbulent state causing the drag to undergo a sudden reduction. These complex phenomenon can be only captured by using highly resolved numerical techniques such as Direct Numerical Simulation (DNS).

In this regards DNS simulations were done for a single falling spherical particle by using the non-Lagrangian fictitious domain method based in-house code developed by Veermani et al, 2007. We could accurately predict the terminal settling velocity, drag coefficients and lift coefficients, however the streamlines and azimuthal vortices couldn't be obtained.Post processing of transverse as well as streamwise velocity data was done using MATLAB code of Fast Fourier Transfer (FFT) to find the vortex shedding frequency in terms of the non-dimensional frequency Strouhal number Energy Spectra for 3D flow past square cylinder was done using LES Model and energy spectra was obtained as shown in Figure 1 below.

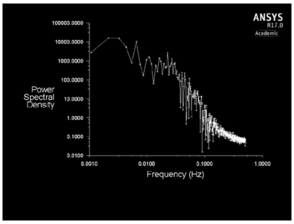



Figure 1: Energy Spectra for Flow Past Square Cylinder of 10mm

Swapnil Rameshrao Chaudhari

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|---|---|---|
| **Project** | : | Transport of actinides and fission products across hollow fibre supported liquid membrane (HFSLM) |
| **Designation** | : | PhD (Tech) 4th Year in Chemical Engineering |
| **PhD Registered Topic** | : | Studies in advanced membrane separation processes |
| **Supervisor from ICT** | : | Prof. (Dr.) Anand V. Patwardhan |
| **Co-Investigator** | : | Prof. (Dr.) Ashwin W. Patwardhan |
| **Supervisor from BARC** | : | Dr. P. K. Mohapatra |

**Current Status of the Project Work:** Extraction of Cobalt, Zinc, Strontium, and Neodymium has been performed through hollow fibre supported liquid membrane (HFSLM). The study of extraction of individual Lead and Cadmium ions using both flat sheet and hollow fibre supported liquid membrane has been completed. The set up to study the above experiment has been already installed in an institute. Mathematical model was developed to represent transport mechanism in membranes. The model is used to estimate separation efficiencies for different process conditions. This will help in predicting the long term use of the contactors and also scaling up of the process. Currently, the work on transport of Ruthenium through supported liquid membrane is in progress. In future, transport of Europium through supported liquid membrane will be performed.

**Work done during the Year 2016-2017:** During the year 2016-2017, extraction of ruthenium from synthetic solutions has been performed. Ruthenium is found in spent solutions arising from various industries [1]. Membrane based advanced separation technique such as supported liquid membrane (flat sheet and hollow fibre) was used for the concentration and separation of ruthenium. The experimental set-up consists of the feed phase reservoir, strip phase reservoir and flat sheet / hollow fibre membrane. Porous nature of the membrane was used for the impregnation of suitable complexing agent. Equilibrium experiments were performed to find out the optimum concentration of complexing agent. Aliquat® 336 (trioctylmethylammonium chloride) was found to have suitable extraction capacity for the extraction of ruthenium from chloride media [2]. Effect of Aliquat 336 concentration was studied with 100 ppm of ruthenium chloride in 1 M HCl solution as feed. A mixture of (90/10%) n-dodecane and 1-decanol was used as diluent. 0.5 M Aliquat 336 concentration was found to be optimum. HCl of various concentrations was used as stripping agent for the removal of ruthenium from supported liquid membrane. Quantification of ruthenium was done using ICP-OES Spectrometer (Model No. iCAP 6000 series Thermo SCIENTIFIC) at 267.8 nm. Transport study was done with both flat sheet and hollow fibre supported liquid membrane. Transport of ruthenium was more in flat sheet (flux:$1.07 \times 10^{-3}$ mol m$^{-2}$ sec$^{-1}$) as compare to the hollow fibre (flux: $6.20 \times 10^{-4}$ mol m$^{-2}$ sec$^{-1}$). The above finding was supported by the difference in the pore size of flat sheet (200 nm) and hollow fibre (30 nm) membrane.

*Keywords:* Membrane; Ruthenium; Aliquat 336, Extraction

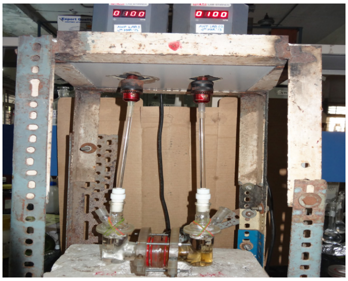
**References:**

[1] Swain et al., 2013. Separation and recovery of ruthenium: a review

[2] Panigrahi et al., 2013. Extraction of ruthenium using both tertiary and quaternary amine from chloride media

**Experimental set-up photographs**

*Photograph 1: Flat sheet supported liquid membrane*



*Photograph 2: Hollow fiber supported liquid membrane*

*Analytical Instrument (ICP-OES) photograph*

***Presentations (Oral / Poster) in Conferences / Workshops / Seminars***

Swapnil R. Chaudhari, P Lakshmi Narayan Patro, Anand V. Patwardhan; "Transport of Ruthenium through Supported Liquid Membrane" delivered ORAL presentation at International Conference on Membrane Technology and its Applications (MEMSEP -2017) at National Institute of Technology, Tiruchirappalli, India during February 21-23, 2017

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Gaikwad Ganesh Arjun

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| **Project** | : | Conjugation and radiolabeling of various Nanoplatforms for image guided theranostic applications |
| **Supervisor from ICT** | : | Dr. R. D. Jain |
| **Principle Collaborator** | : | Dr. Ruble Chakravarty |
| **Principle Collaborator** | : | Dr. Sudipta Chakravarty |

**Summary:**

The conventional systemic drug delivery approaches cannot completely remove the competent cancer cells without surpassing the toxicity limits to normal tissues. Thus more efficient and safer therapy is an urgent need of the hour. Imaging guidance is essential in order to mark the tumor site and to monitor the treatment via imaging modalities or by a stand-alone tool integrating imaging and therapeutic capabilities. The fundamental aim of this project is to develop an approach to provide basic support for the optimization of innovative diagnostic and therapeutic strategies through radioisotopes, that could contribute to emerging concepts in the field of "personalized medicine". Also, nuclear imaging approaches such as single photon emission computed tomography (SPECT) and positron emission tomography (PET) can play an increasingly important and revolutionizing role in disease management. Synergistic use of SPECT/PET imaging and targeted drug delivery approaches provides unique opportunities in a relatively new area called 'image-guided drug delivery'

(IGDD). The objectives of present project are :

- Engineering of various polymeric and metal nano-platforms through continuous process
- Development of radio-labelling strategies for nano-platforms, and applying these strategies to radiolabel the nano-platforms with radioisotopes.
- Structural and functional and characterization of radio-labelled nano-conjugates.
- Optimization of the parameters of the process used for synthesis of nano-conjugates for large scale synthesis of nano-platforms and rapid labelling technology
- Cellular evaluation, toxicity studies and bio distribution of the radio-labelled nano-platforms.
- Pre-clinical evaluation studies of the radio-labelled nano-conjugates.

Design and fabrication of micromixer for continuous synthesis of Chitosan oligosaccharide nanoparticles has been done. Continuous synthesis of Chitosan oligosaccharide nanoparticles using micromixer is under process. Microreactor designing for metal nanoparticle synthesis has been done and fabrication of the same is under process. Moreover, colloidal PEG functionalized silver nanoparticles synthesis by batch process is done. Continuous system for nanoparticle synthesis is under development.

Anita Sharma

**Project** : Synthesis and Characterization of Boron and Nitrogen-doped CNTs

**Supervisor from ICT** : Prof. Ashwin Patwardhan

**Co-Principal Investigator** : Prof. J. B. Joshi

**Introduction**

Heteroatom doping in the lattice of carbon nanotubes (CNTs) using chemical vapour deposition (CVD), has been an area of research since a long time. Atoms, such as Nitrogen (N), Boron (B) or combination of both have been extensively doped for better reactivity of the CNTs to be used in high end applications Doping can be carried out in many ways but CVD is one of simplest and most efficient methods which can help in producing appreciable quantities of CNTs at low temperatures (450oC -850oC) Nitrogen and Boron are the most commonly doped elements in the lattices of the CNTs because the size of these two elements is comparable with carbon, which helps in formation of strong bonds. The research till now has been confined to study of, effect of a single parameter on the nature of the doped CNTs formed. The combined effect of variation in different parameters like temperature, partial pressure/concentration of reactants, catalyst concentration, catalyst size and total flow rate of the species, has not yet been deeply studied. The reaction mechanism and the chemical engineering aspect of N-CNTs and B-CNTs have not yet been studied systematically in order to find the rate of formation of N-CNTs and the rate controlling step (s). Though sufficient information is available on the kinetics and large scale production of pristine CNTs,yet it is still missing for N-CNTs and B-CNTs. Thus, understanding of different parameters affecting the growth pattern of N-CNTs and B-CNTs is required to provide a platform for qualitative and quantitative synthesis of N-CNTs. This inculcates a strong need to verify the contribution of each parameter very carefully to fully understand the growth mechanism the doped CNTs.

**Objectives:**

- Production of N-CNTs and B-CNTs at gram scale using chemical vapor deposition in fixed and fluidized bed reactor.
- Understanding the kinetics and mechanism of formation of N-CNTs and B-CNTs for its large scale production
- Utilization of N-CNTs

and B-CNTs for different applications like hydrogen storage, electrochemical studies and catalysis.

**Nitrogen doped Carbon nanotubes (N-CNTs):** N-CNTs were synthesized in fixed and fluidized bed reactors by chemical vapour deposition technique using Imidazole as both carbon and nitrogen source, acetylene as additional carbon source, ferrocene/MgO as a catalyst and Argon as inert gas

From temperature studies it was found out that the activation energy obtained during formation of N-CNTs was around 114.15 kJ/mol, which indicated the presence of surface reaction resistances. Pore sizes of <91 µm of MgO particles were useful in eliminating the pore diffusion resistances. Flow rate of > 400 sccm and catalyst weight of 0.4 to 0.8 g was responsible for eliminating the bulk diffusion resistances and temperature gradient effects. At 950oC, N-CNTs disintegrate due to release of nitrogen gas. The acetylene gas helped in tuning the nitrogen content of the N-CNTs uniformly even if the reaction temperature was kept constant. The nitrogen content was found to be varied from 4.12% to 13.82% for temperature ranging from 600-950oC and partial pressure ranging from 0-0.48 atm. (temperature of 900oC), the nitrogen content varied from 3.73% to 6.52%. The N-CNTs were also synthesized in a fluidized bed reactor using only imidazole. The morphology of N-CNTs was found to be very uniform for a temperature of 850oC. The samples were investigated for utilization in hydrogen storage and it was found that for N-CNTs with good surface area and appreciable nitrogen content the hydrogen storage capacity (room temperature and 50 atm. pressure) improved from 0.02 wt% for bare CNTs to 0.35 wt % for N-CNTs.

**Boron doped Carbon Nanotubes (B-CNTs):** B-CNTs were synthesized in a fixed bed reactor by chemical vapor deposition technique using Acetylene as carbon source, boric acid as boron source, ferrocene/MgO as a catalyst and Argon as an inert gas. The kinetic studies were carried out accordingly as given in **Table 2.** The temperature studies revealed the presence of two different mechanisms governing the reaction at two different temperature ranges. The activation energies for both the reaction rates were found to be 6kJ/mol and 18kJ per/mol respectively. The flow rate of > 2400 sccm and catalyst weight of around 2.4 g could help in eliminating the mass transfer diffusion resistances. The partial pressure studies revealed that the partial pressure of 0.25 atm. of acetylene was best suitable for getting B-CNTs of uniform diameter in appreciable quantities at a temperature of 800oC.