DEPARTMENT OF

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 sec ond 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
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.	Bhavesh Gajbhiye	Thermal hydraulic studies related to coolants for new generation reactants	ICT, Mumbai	M. Chem. Eng	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

RESEARCH STUDENT:

BHAVESH D. GAJBHIYE

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

New generation nuclear power plants are currently being developed to be, highly economical, safe, produce a minimal waste and produce electricity and hydrogen. An important feature of these reactors will be the use of coolants to transfer the heat from the high temperature heat source to the hydrogen production plant at temperatures much higher (750°C) than that being used in current generation reactors (550°C). For a reliable design of heat transfer loop, it is necessary to characterise the thermal hydraulic performance of molten salt.

High temperature heat transfer experiments with molten salts is a very challenging task. Hence, heat transfer experiments with thermic fluid (Thermia-B) were carried out to test the experimental set-up and the experimental results were validated with CFD results and various heat transfer correlations obtained from literature. CFD of molten salts has also been carried out. Soon heat transfer experiments with molten salts will be carried out.

Molten salt flow loop

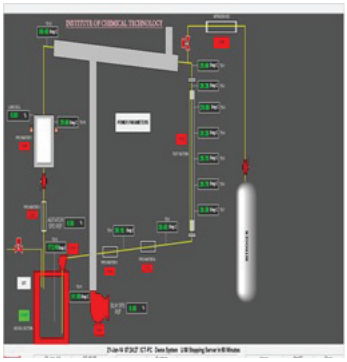


Figure1: Experimental set-up for heat transfer studies along with SCADA image

EQUIPMENTS PURCHASED

1. 2 High temperature fire protection suits with 2 pairs of high temperature aluminized shoes, 1 aluminized hood. 1 Pair of high temperature aluminized gloves.- Rs. 22000.
2. 2 Pair of Kevlar gloves- Rs. 2000 Approx.

Figure 2: High temperature fire protection suit for safety

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, Department of Chemical Technology, Institute of Chemical Technology Mumbai

Co-Investigator: Dr. D. Mandal, Head, AMMD, Chemical Engineering Division, Bhabha Atomic Research Centre Trombay, Mumbai

The primary source of energy for our planet is the sunlight. The energy from sun is derived from the fusion reaction. Imitation of this process in controlled manner is challenging task and if successful, will provide with practically unending source of energy. The theoretical designs are under experimental investigation for their operational feasibility, efficiency, safety and scalability. One of the problem lies in efficient transport of the heat generated in the core of the reactor. Scientists are trying to couple this removal of heat with the in-situ production of feed for the fusion reaction, so that the whole process becomes self-sufficient and efficient.

We are working on development of Packed Fluidization systems. Packed fluidization tries to couple this production of Hydrogen isotopes and removal of 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. 3D-CFD modeling of the system is done to understand the hydrodynamics and heat transfer through the packed bed. Effect of external heating on minimum fluidization velocity and the effective thermal conductivity is studied. It is found that developed and validated CFD model can give the response of the system in fairly accurate quantum.

Ongoing Work

1. CFD modeling to predict minimum fluidization velocity at different temperatures
2. CFD Simulations to predict the effective thermal conductivity Packed and fluidized Bed
3. ANN Analysis of experimental and literature data for prediction of Keff
4. Analysis of different packing algorithm to generate packed bed geometry
5. CFD simulations to predict Minimum Fluidization Velocity in Packed Fluidized Bed
6. CFD modeling to predict the Effective thermal conductivity in Packed Fluidized Bed

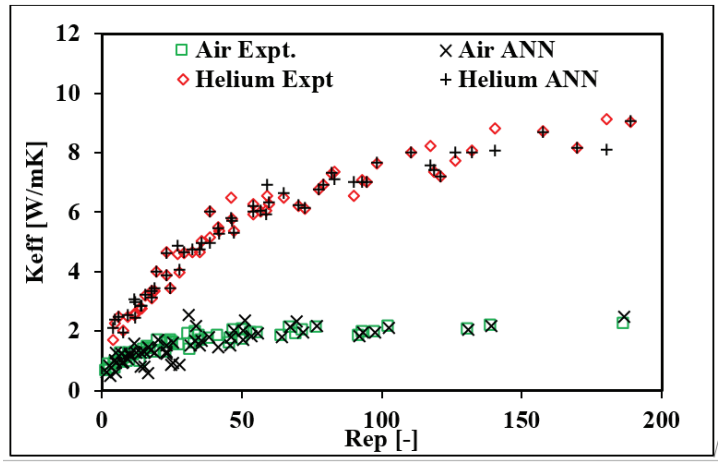


Figure 1: Effective thermal conductivity of packed bed of Li2TiO3 with air and helium as fluid media

ZAKIR HUSAIN MOHAMMED YUSUF

Project : Modeling and simulation of solid fuel burning devices.
Supervisor from ICT : Prof. A. B. Pandit
Co-Investigator : Prof. J. B. Joshi

Energy has a vital impact on the economic and social development of the country. Energy sources like fuelwood, charcoal, dung etc. were the only source of energy used for almost all applications in the earlier days. In the last three centuries, fossil fuel such as coal, oil, and gas have become the major source of energy. However, it is estimated that the world's 75 % population still relies on the traditional source of energy for their requirements even today. The majority of the population are from developing nations. In particular, the domestic sector heavily relies on the traditional source of energy, mainly for cooking. The rural energy demand for cooking in developing countries are still supplied through biomass-based fuels. India has a huge population (1095 million in 2005) and about 30 % of this resides in urban areas. Rural households depend on biomass for almost 85 % of their cooking needs while LPG (Liquefied Petroleum Gas) meets 56 % of this need in urban households. Urban households, which make up less than 30% of India's population, account for 75% of India's residential demand for LPG. Rural households account for 92% of India's residential use of biomass. Noting that the energy efficiencies in the conventional burning/cooking process are less than 25 %, if proper attention is paid in this area, it will result in helping prevent the environment through reducing CO2 emissions.

Solid fuel includes biomass fuels such as wood, charcoal, crop residues and animal dung remain, the most common sources of household energy supply in most of the developing world. They account for about one-third of total energy consumption in developing countries as a whole, and nearly 90 percent in some of the least developed countries (Kartha and Larson 2000). Traditionally, these solid fuels have been burned with poor combustion efficiency under poorly ventilated conditions, such as the three-stone fire inside a hut. This has resulted in a host of problems, including damage to human health from indoor air pollution, pressure on natural ecosystems from fuel gathering, and excessive time spent on fuel collection by the poor at the expense of time for income generation, education, and childcare and so on.

It is possible to burn biomass

(wood and agricultural residues) quite cleanly, producing mostly carbon dioxide and water, but such conditions are difficult to achieve with small-scale inexpensive stoves. Studies in India and China, for example, show that the percentage of fuel carbon fully burned to carbon dioxide is typically only 90 %, with some fuel/stove combinations only achieving 80 %. The remaining 10 to 20 % is diverted into products of incomplete combustion-primarily carbon monoxide, particulate matter including benzene, 1, 3-butadiene, formaldehyde, polyaromatic hydrocarbons, and many other compounds posing health hazards.

The impact of these conditions on the life expectancy and quality of life of the women involved is severe. The danger to their physical health can be reduced through better-designed stoves. Biomass embraces a wide variety of fuels with varying elemental composition. Due to the diversity of biomass fuels, a specific biomass combustor must be optimized with respect to a certain type of fuel, or a group of fuels with similar combustion characteristics. This optimization is focused on achieving the highest possible combustion efficiency and thermal efficiency to increase the cost-effectiveness of the biomass combustor.

Definition of problem

It was reported in 2002 that two billion people worldwide still depend on solid fuels like firewood, agriculture residue and coal for cooking food. This practice results in a high level of indoor air pollution [Energy for cooking in developing countries].

Objectives:

The objective of this study is to determine possible methods of applying technology that exists in the modern developed world to assist in solving the problem of indoor air pollution and low efficiency of the cook stove. Furthermore to produce conclusive evidence that CFD can be used in a viable manner to assist in the development of smokeless cookstoves with higher heating efficiency. Our research work mainly addresses this issue by showing the effect of geometrical variations on hydrodynamic and combustion parameters.

Major Physical/Technical Progress Achieved Till End of June 2018:

Part 1: Pyrolysis of biomass pellets at different temperature ranging from 200 °C – 600 °C in the batch reactor has been completed. Pyrolysis products like gasses, liquid and solids are analyzed. Flowing analysis techniques were used for the pyrolysis products.

Gas: Gas Chromatography

Liquid: HPLC, GC-MS

Solid residue: IR, SEM, TEM, XRD, Zeta sizer etc.

Part 2: To study the pressure, velocity and uniformity of air distribution in the solid fuel burning device (i.e. Eco-Biomass Cook Stove) the flowing simulations of has been completed.

A) Simulation of empty solid fuel burning device (i.e. Eco-Biomass Cook Stove).
B) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with a grate at the bottom.
C) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with an orifice plate.
D) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with an orifice Plate and grate at the bottom.

Major Physical/ Technical Progress Achieved During July 2017-June 2018:

To study the pressure, velocity and uniformity distribution of air in the solid fuel burning device (i.e. Eco-Biomass Stove from Sanjay Technoplast, Aurangabad) the flowing simulations of has been completed.

A) Simulation of empty solid fuel burning device (i.e. Eco-Biomass Cook Stove).
B) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with a grate at the bottom.
C) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with an orifice plate.
D) Simulation of solid fuel burning device (i.e. Eco-Biomass Cook Stove) with an orifice Plate and grate at the bottom.

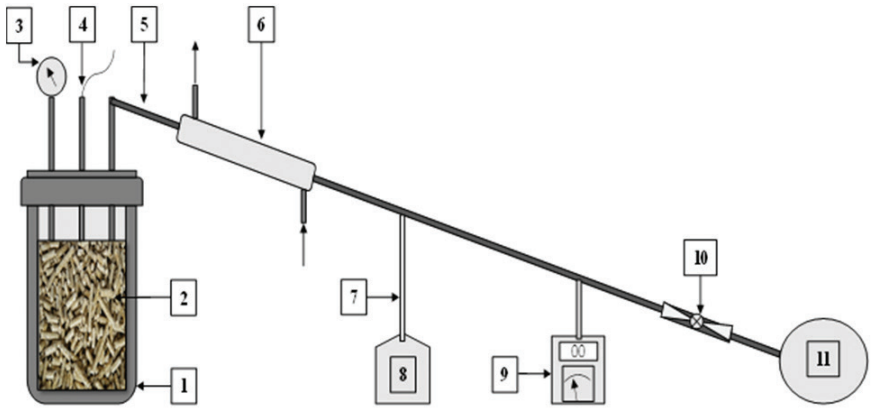


Figure 1: Experimental setup for pyrolysis of biomass pellets

(1) SS 316 autoclave; (2) Biomass pellets; (3) Pressure gauge; (4) K-type temperature sensor; (5) Gas outlet tube; (6) Water condenser; (7) Outlet for condensable gasses; (8) Liquid product collector; (9) Gas flow meter; (10) Gas stopper; (11) Gas balloon

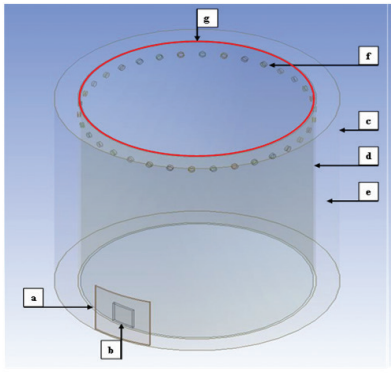


Figure 2.1 Empty eco biomass Cookstove

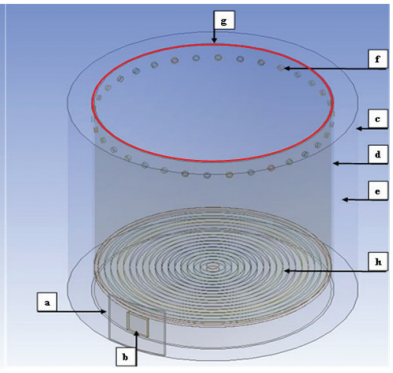


Figure 2.2 Eco Biomass cookstove with grate

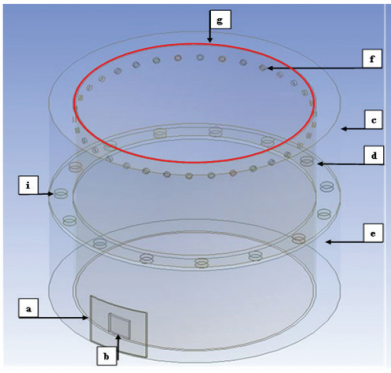


Figure 2.3 Eco biomass cookstove with orifice

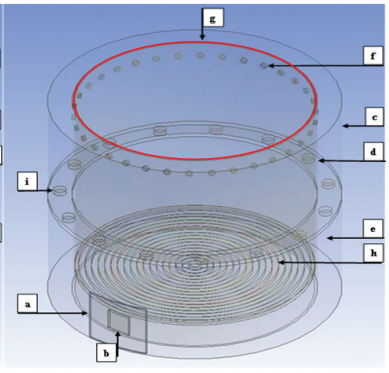
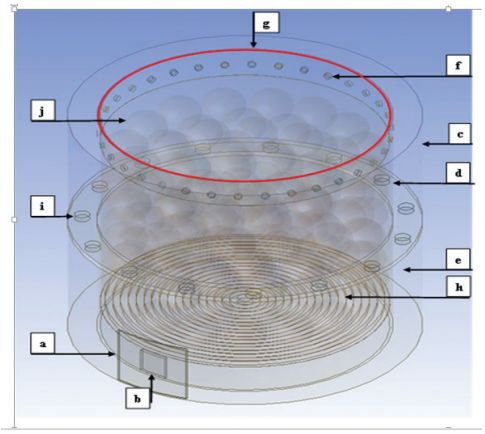


Figure 2.4 Eco biomass bookstove with grate and orifice



[a] Inlet for air, square cut on outer cylinder body (50mmx50mm)
[b] Square cut on inner cylinder body (20mmx20mm)
[c] Outer cylinder (□=230mm, H=210mm)
[d] Inner cylinder (□=190mm, H=210mm)
[e] Annulus space (40mm)
[f] Secondary holes (□=5mm, 34 nos)
[g] Outlet
[h] Grate at the bottom
[i] Orifice plate in annulus space
[j] Packed bed (□=20mm, void=0.5)

Figure 2.5 Eco biomass cookstove with grate, orifice and packed bed

MR. NILESH HENDRE

Project : Computational Fluid Dynamics Modeling of Asymmetric Rotating Disc Contactors
Supervisor from ICT : Prof. V.G. Gaikar

Hydrodynamic performance of lab scale ARDC and ARIC (4" I.D.) was studied. Based on the available experimental data, generalized correlations were developed for the prediction of drop size and holdup in ARIC and ARDC. The average error in the prediction of drop size and hold up using the developed correlations are 18% and 14%, respectively. Guidelines for the scale up of ARIC (12") were developed based on CFD simulations and the geometrical parameters were optimized. Mass transfer performance of 12" ARIC was checked at different operating conditions. The performance was found satisfactory as predicted. Further CFD-PBM simulations of ARDC and ARIC have been carried out. Effect of different breakage and coalescence kernels on drop size distribution was studied. Luo and Svendsen model has been found to over-predict the drop size whereas reducing the coalescence rate slightly reduced the drop size. The error in prediction of drop size was found to be more than 50%. Breakage and coalescence model of Coulvoglou and Tavlrides has been found to predict drop size and holdup satisfactorily.

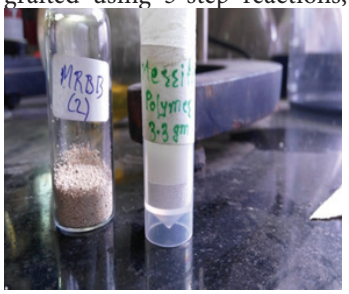
Pilot scale ARIC (12")

SWAPNIL RAJPUT

Project : Development of grafted resins and membranes (extractants) for precious metals
Supervisor from ICT : Prof. Anand V. Patwardhan

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 but are also suitable for continuous column mode operations. Their scale up is under study, to regulate engineering parameters which might affect the final grain size. Simultaneously, similar chemistry was used to graft diglycolamide functionality over dendritic support. New dendrimers have been synthesized and their grafting was tried to not only make them hydrophobic but also an efficient cheap extractant which can suffice existing TODGA in terms of robustness and higher partition coefficients. One extractant, out of 12 synthesized was found to fulfill above criteria and its scale up is under study.

SHASHANK SURENDRA TIWARI

Project : Direct Numerical Simulation of Flow Patterns in Multiparticle Systems
Supervisor from ICT : Prof. Ashwin W. Patwardhan
Co-Investigator: Prof. J. B. Joshi, Emeritus Professor, Homi Bhabha National Institute, Mumbai

Multiparticle flows are encountered in a number of naturally occurring phenomenon as well as in artificially designed equipment. The rapid variations in the flow patterns in the fluid due to the translational and rotational motion of the particles or that of the fluid across stationary particles, has been a fundamental area of research in fluid mechanics. 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 the boundary layer 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) or Large Eddy Simulation (LES) or by using high fidelity flow visualization techniques like Particle Image Velocimetry (PIV), Schilerian Shadowgraphy, Laser Doppler Anemometry (LDA), and Hot Film Anemometry (HFA).

Highlights of the Work done in 2017-18

1. Two review papers were communicated on the topic of flow past a stationary sphere. The first one comprising of the recent advances in computational models, experimental techniques and post processing for characterisation of turbulence in three dimensional wake flows. The second one addressing ocuses on the regime mapping for flow over a stationary rigid particle from Re = 1 to 106.
2. Direct Numerical Simulation were performed for 100 < Re < 1000, and flow structures were examined. New insights with respect to a new dominant frequency mode was determined. The effects of this dominating frequency on force coefficients were evaluated and a manuscript from it was communicated.

3. DNS simulations were done to investigate the mass transfer effects for multiparticle system. Packed beds of varying D/d ratios were investigated to study the effects of Sc varying from 1 to 1000 at Re ranging from 1 to 100. Representative snapshots of different active particles for D/d = 6 has been shown in Figure 1.
4. DNS simulations have been carried out in the critical Re regime to predict the drag crisis. The drag coefficient are found to be in line with the experimentally reported values of Schlichting et al. (1968) as shown in Figure 2.

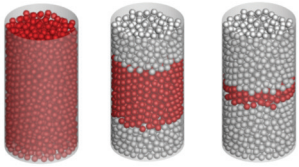


Figure1: Representative snapshots of the packed bed column (a) X/L = 1 (b) X/L = 0.5 and (c) X/L 0.125.

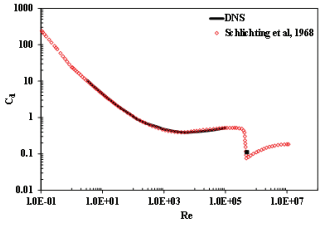


Figure 2: Validation study of drag coefficient at varying Re against experimentally reported values of Schlichting et al. (1968)

Comments

My PhD research work is an effort in better understanding of the physics of turbulent flows with the aid of high fidelity Direct Numerical Simulations. This project is a small step in the direction of developing reliable design and scale up procedures for multiparticle reactors based on rational approach. Multiparticle flows are encountered on a wide scale in chemical engineering industries. The design procedures of such reactors even today is an art rather than science. The Re at which these multiparticle reactions are carried out varies over a wide range. The physics involved in such multiparticle flows, traces back to the fundamental of single particle flows which is still not completely understood. Thus in the present research work, we begin investigating flow of fluid over a single particle and then extend the study up to multiparticle systems with a single objective of understanding turbulence.

SARVESH SANJAY SABNIS

Project Title: Improved Crystallization and Cleaning Using Ultrasound (2017-18)
Supervisor from ICT : Dr Parag R. Gogate, Department of Chemical Technology Institute of Chemical Technology, Mumbai

Crystalline deposits on hot surfaces is a major problem in heat exchange equipment used in thermal desalination operations. For this, a heat exchanger has been designed and set up to study the extent of fouling on titanium tube due to CaSO4 solution at varying temperatures and flow rates. Fouling resulted in 25% - 30% drop in the heat transfer coefficient. The concentration of fouled CaSO4 was measured using both titration by EDTA method and UV spectrophotometer. The next step is to incorporate ultrasonic device for crystallizing out CaSO4 and other salts from simulated seawater and minimize fouling in the heat exchanger as shown in the figure below.

Also a commercial polymer additive was crystallized using ultrasound assisted antisolvent crystallization. The results obtained were promising as the reduction in size was found to be 150% than that of the original sample without compromising on its

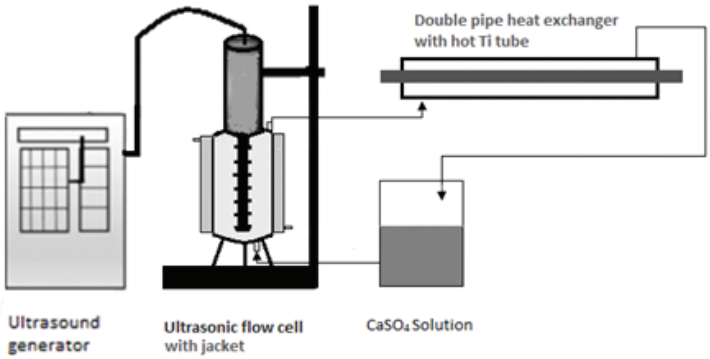


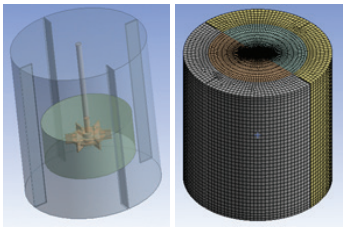
Figure 1: Schematic of ultrasonic treatment of CaSO4 before heat exchange equipment

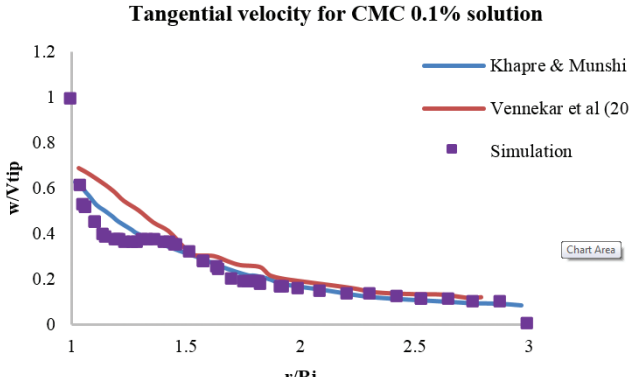
crystallinity. Size reduction of the additive is important for from the point of view of uniform dispersion in the host polymer. Scale-up prospects were also explored using an ultrasonic bath and these results were also promising.

SHRUTI HINGE

Project Title:
Cfd Modeling of Gas-Liquid Stirred Tank Reactors And Fermenters
Research Supervisor : Prof. A. W. Patwardhanm Professor, Department of Chemical Engineering Institute of Chemical Technology, Mumbai

Computational fluid dynamics (CFD) is a powerful tool used to solve complex mathematical models of fluid dynamics using computers. With a few assumptions, this method can describe the complete flow field for all the variables, even for complex design configurations. Predicted flow field can give insight into the reactor. This can be implemented to reactor design at less cost, with lower risk and without need to carry out experiments. CFD can be a useful tool to design stirred tank reactors and fermenters and improve its performance using mathematical and computational modeling method. In the present work, simulations were performed using Fluent 18.0 as a CFD tool. Geometry construction and meshing was carried out with Ansys 18.0. The single phase simulations have been carried out to reproduce the data reported in the literature. The work by Deglon and Meyer (2006) and Joshi et al. (2011) was reproduced for Newtonian fluid using the standard *k*-ε model in a standard stirred tank. Further, a study by Khapre and Munshi (2015) was reproduced for Newtonian and non-Newtonian power law fluids using the realisable *k*-ε model in a standard stirred tank with Rushton turbine and CFD model was validated.



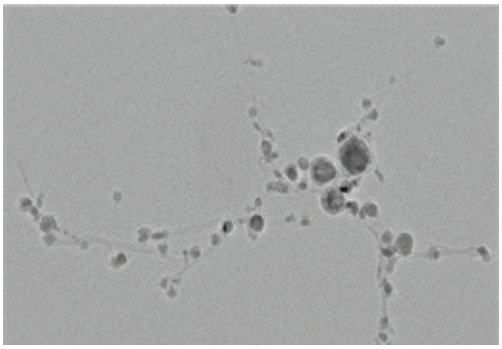


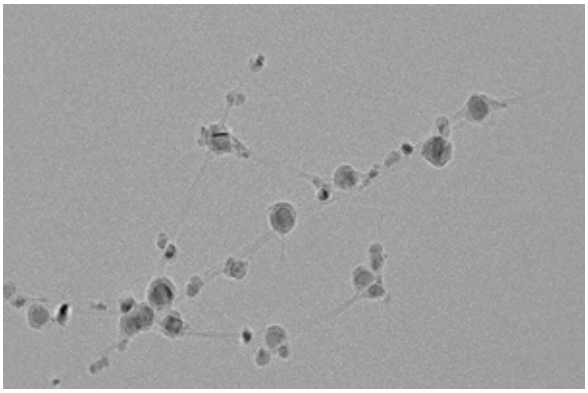
SHRILEKHA VIJAYSINH SAWANT

Project : Synthesis and modification of Carbon nanotubes: Modeling, Experimentation and Applications
Supervisor from ICT : Prof. Ashwin Patwardhan
Co-Investigator : Prof. J. B. Joshi,
Synthesis of modified carbon nanotubes

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 (H3BO3), trimethyl borate B(OCH3)3 as precursor. Boron atoms in CNTs act as electron acceptors producing p-type CNTs. Therefore for characterization, Field emission spectroscopy and Raman spectroscopy are highly used. The synthesized BCNTs TEM micrographs are given below





TUKARAM UDHAVRAO SHINDE

Project : Mathematical modeling of the gas centrifugal separator

Supervisor from ICT : Dr. V. H. Dalvi

The project aim is to mathematical modeling of the gas centrifugal separator and determines the order of magnitude of the maximum achievable separation for gas using a gas centrifugal separator. There are various problems in gas centrifuge design, the gas dynamics of the gas centrifuge is not well understood and have very low literature available. Development of well-matured model is necessary for further development of gas centrifuge. To solve mathematics there is failure and limitation to solving the centrifugal separator problem due to the limitation of compressible turbulence modeling in numerical software like Ansys and OpenFoam. We are trying to develop a new novel meshfree Lagrangian – Eulerian hybrid method using voronoi tessellation to solve and mature understanding of gas dynamics of the gas centrifugal separator. The objective of present work to study the fluid flow phenomena using voronoi tessellation, where conserved quantity will be solved by Langarigain approach and dissipation phenomenon solved by Eulerian approach. Voronoi cell will be used in Lagrangian approach to discretize the partial differential equation and solve them in novel mesh-free manner. Suitably for incorporating the advanced thermodynamics on the same platform. Also, a development of suitable partial differential equation for handling the generalize boundary conditions over Voronoi tessellation for gas dynamics phenomena. Above algorithm is based on python programing language code to implement the algorithm.

1. Trying to simulate above algorithm in simple cases like a gas flow in the pipe.
2. Validation of above algorithm done by comparing results with CFD simulations.
3. Currently facing problems over wall boundary condition for gas flow.

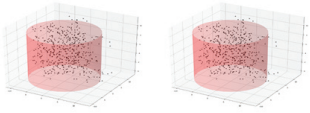


Figure 2 Simulating algorithm for gas flow in the pipe

VAISHNAVI PABBISETTY

Project : Graphene based high performance materials for desalination (2018)
Supervisor from ICT : Dr. Parag Nemade, Department of Chemical Technology Institute of Chemical Technology, 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.
The following work has been done till now:

- Literature survey on synthesis of graphene by various chemical and electrochemical methods, synthesis of graphene oxide, graphene based membranes.
- Synthesized Graphene oxide by Hummers method
- Synthesized Graphene by electrochemical exfoliation
- Characterization of the graphene and graphene oxide synthesized by using above methods
- Preparation of graphene based membranes
- After comparing the Raman spectroscopy of the samples synthesized by above methods it has been concluded that Graphene synthesized by Electrochemical exfoliation has lesser defects and lesser number of layers compared to the one synthesized by Hummers method.

VIKRAM VIJAY BANAKAR

Project Title: Improved process for CaSO4 crystallization in concentrated brine Using Ultrasound (2017-2018)
Supervisor from ICT : Dr Parag R. Gogate, Department of Chemical Technology, Institute of Chemical Technology, Mumbai

The formation of crystalline deposits on the heat transfer surfaces is one of the main problems in thermal desalination processes. In evaporation of sea water, various salts will precipitate in a certain order depending on operating temperature, pressure, ionic strength of solution, etc. The scale deposits are formed from those salts whose solubilities are generally limited and in most instances decrease with increasing temperature e.g. Calcium sulfates (gypsum, hemihydrate and anhydrite) and calcium carbonate.

Depending on operating conditions, the deposition process can be diffusion or reaction controlled, or a combination of both. Based on a careful literature survey, Fouling experiments were carried out to determine how process variables such as surface temperature and velocity affect the initial fouling rates of calcium sulphate scaling. To carry out Fouling experiments the double pipe heat exchanger was designed which was made of Titanium tube as inner pipe and PMMA pipe as outer pipe as shown in fig 1 .To know the extent of CaSO4 deposited, analytical methods like standard EDTA method to calculate calcium ion concentration and photo spectrometer method for sulphate determination were optimized. Fouling reduced the heat transfer coefficient by 25-30% .To reduce fouling it is planned to incorporate ultrasound to crystal out CaSO4 before it fouls the heating surface into the system.

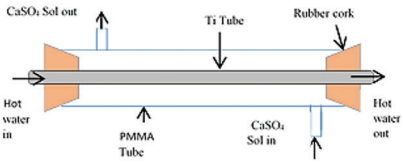
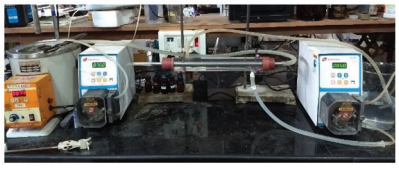


Fig.1: [a] Schematic of Double pipe Heat Exchanger



[b] Double pipe Heat Exchanger set up

PRATIKSHA MADHUKAR BIRANJE

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

Supervisor from ICT : Prof. Ashwin W. Patwardhan

Co-Investigator: Dr. J. B. Joshi

Graphene is a 2-D material. Graphene is a hexagonal structure consisting of sp2 hybridized carbon atoms, described as the 'mother' of all graphitic carbon materials due to it essentially being the building block for carbon nanotubes, effectively 'rolled up' graphene sheets and graphite, stacked graphene sheets held together by strong Vander Waal's forces. The main focus of this study is on graphene synthesis. Characterization methods are Raman spectroscopy, thermogravimetric analysis (TGA), SEM, TEM, X-ray diffraction (XRD).

Highlights of the Work Done in 2017:

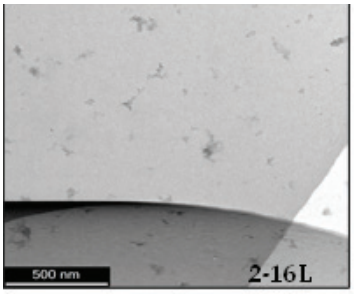
1. Graphene oxide synthesized by electrochemical exfoliation technique. An electric field that gets generated between two electrodes affects the exfoliation pattern. A lack of area coverage of anode by a cathode resulted into inefficient graphite exfoliation.
2. The new design of setup was able to remove the errors or lacunae of previous geometry. A setup was designed to facilitate a continuous process.
3. Graphite with density 1.82 was used as anode.
4. The parameters that affect exfoliation rate were determined.

Comments:

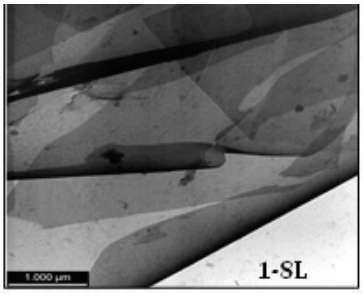
An electrochemical exfoliation is able to offer in-situ functionalization of graphene. The graphene oxide was synthesized using electrochemical exfoliation of graphite. A graphite discs with different bulk densities were exfoliated. A facile system was developed such that a continuous exfoliation and re-exfoliation of graphite was achieved. The parameter optimization like, ratio of electrolyte constituent H2SO4 and NaOH, and area of flux were attained to obtain a continuous synthesis of graphene oxide.

A structural and chemical characterization was done using XRD, TEM, Raman and XPS. TEM images have shown the effect of synthesis environment on GO sheet dimension. Electron transmission could successfully observe the contrast in transparency of single separate sheet and dark region due to overlapping of multiple few layers GO sheet. A characteristic peak broadening and shifting was observed in Raman Spectrum. XPS shows the varying C/O ratio as an effect of electrolyte composition. This method functionalizes graphene and helps in forming a stable dispersion in ethyl alcohol and water.

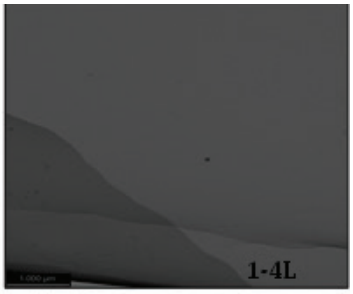
Transmission Electron Microscope (TEM):



SO_4:Na≈1



SO_4:Na≈1.6



SO_4:Na≈2

Proposed Work in 2018:

1. To study a effect of ampere upon exfoliation
2. Temperature study 30°C, 40°C, 50°C, 60°C
3. Ultrasonication / Stirring(RPM) study
4. Polymer composite

AMOL VILAS GANJARE

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

Supervisor from ICT : Prof. A. V.Patwardhan

Gravity settlers are used for the separation of suspension into two phases. The common applications are treatment of urban wastewater treatment, algal dewatering, microalgae harvesting, separation of oil water emulsion, and potable water treatment. The effective water treatment involves a complex system of physical, chemical and biological processes in a hydrodynamic environment. To optimize this, we need to understand the relationships between the things involving in the process. The optimization can lead to development of new design strategies and criteria which will result in greater efficiency and reduction in capital, energy, and chemical input.

The comparison of turbulence models for the gravity settling is aimed for the single phase. The evaluation of the model performance is made by comparing the velocity field and turbulent kinetic energy predicted by the models with the experimental data. It is been observed that the low Reynolds number models work well for the gravity settler and predict better than the standard k epsilon model. The pathline prediction with different models show the extent of the recirculation happening in the settling tank. The low Reynolds number models are showing that the recirculation zone is more as compared to the standard k epsilon model. The Abid model predictions are better than other models. The comparison between the other turbulence properties also shows the same behavior.

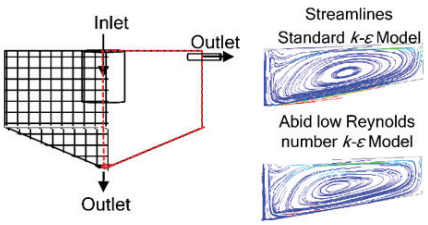
Highlights of work done in this year

1. Developing the geometry and Meshing for rectangular and circular settling tank.
2. Single phase simulations of the developed geometries.
3. Improving the mesh and boundary conditions according to the flow characteristics.
4. Mesh indecency study.
5. Study of different turbulence models.
6. Comparing outcomes of different turbulence models studied with the available experimental data.
7. Interpretation of results obtained from the simulations.

The lab scale model is setup containing the gravity settler and the mixing tank for continues constant concentration feed to the gravity settler. Various materials like calcium carbonate, sand, and gypsum will be used for the settling. The flow conditions, loading and the percent removal of the solid from the suspended media are being studied for the optimize performance of the settlers. Once the experimental conditions are optimized the CFD model for the same will be developed.

Proposed work in next Year

1. Detailed study of turbulence model for settler application for two phase simulations.
2. Two phase experiments for the settling of the particles.
3. Carrying out two phase simulations for different geometrical and operational parameters in the modelling.
4. Simulations and validation of the lab setup for two phase conditions.
5. Study flocculation in the lab setup and developing CFD model for flocculation in the gravity settler.



Velocity pathlines predictions with Model Settler

Experimental Setup of Gravity

CHAITANYA DILEEP MOHOLKAR

Project : Improved process for CaSO4 crystallization in Concentrated brine using ultrasound – CFD Modeling

Supervisor from ICT :
Prof. P. R. Gogate, Professor, Department of Chemical Engineer Institute of Chemical Technology, Mumbai

It is proposed to see the effect of ultrasound to improve the process of crystallization of CaSO4 from the feed and also evaluates the performance in comparison to the existing approach of seeding. The main objective of this project is to develop CFD model for Ultrasound assisted crystallization and validate the model using experimental Data. Project will include proper understanding of Physics of Sono-crystallization based on which basic conservation equations will be written and the set of assumptions along with theoretical framework used to develop them. Simulations will be carried out in order to study various aspects of crystallization such as seeding, crystal growth etc. and gain insight into the subject making use of Post processing abilities that CFD presents.

Highlights of the Work Done in 2018

1. Literature review was carried out in order to understand the bubble dynamics in Acoustic Cavitation. Objective of this exercise is to develop the ability to write conservation equations for the same with proper understanding of the physics.
2. Study of computational fluid dynamics principles and the basics was carried out in order to gain an understanding of the subject.
3. Partially learned CFD software ANSYS and OpenFOAM. Few Tutorials for Geometry creation and Meshing are completed. Folder structure in OpenFOAM is well understood and few tutorials were completed on OpenFOAM.
4. 4. Tutorials were executed to study and understand how to write User Defined Functions (UDF) in FLUENT, precursor for writing UDF for Acoustic Pressure Source.

Proposed Work in 2019

1. To write UDF for acoustic pressure source in FLUENT. Simulate and study the Pressure profiles and determine the effective area of cavitation.
2. Heat Transfer studies in double pipe heat exchanger system.
3. Study and simulate Population Balance Model (PBM) for study of cavities.

SHREERANG DATTATRAY DATAR

Project : Graphene based high Performance Materials for water desalination

Name & Address of PI : Dr. Neetu Jha, Department of Physics, Institute of Chemical Technology, Mumbai
Name of CI : Dr. Parag Nemade
Name of PC : Dr. Soumitra Kar
Name of Co- PC: Dr. A. K. Ghosh

Lowering the cost of recovery of potable water from saline solutions is necessary to address water shortages as well as to achieve zero discharge for industrial effluents.

We propose to develop next generation desalination technologies using a three pronged approach based on graphene based materials to lower the cost of desalination. First approach is experimental scale, high risk high reward scheme for development of all-graphene membrane at a scale of 100 cm2. In the second approach, we are developing capacitive desalination setup for use with dilute feeds as an alternative for ion exchange technologies, at the scale of (Capacity: 50 ml and electrosorption capacity of 25 mg/g). In the third approach, we will develop and evaluate graphene based nanocomposite thin film reverse osmosis membranes. Leveraging the expertise of Desalination group at BARC, 2512 sized spiral modules, used in household RO filters, with nanocomposite membranes will be produced.

Highlights of the Work Done in 2018:

Graphene oxide were prepared by Hummer's method.

Synthesis of reduced graphene oxide was done by using solar energy.

Fabrication of Flow through capacitive deionization (CDI) set up was done.

Comments:

Hummer's method is one of the most popular graphene oxide (GO) synthesis methods. Graphene oxide was prepared by this method and characterized by X-ray Diffraction spectroscopy (XRD). Figure 1 represents XRD of GO , in which sharp peak at 11o depicts there is formation of GO.

Synthesis of reduced graphene oxide (rGO) was done by using solar energy.

Fabrication of Flow through capacitive deionization (CDI) set up was done. Figure 2 represents the set up. The set up consists of two acrylic plates of dimension (10 cm*10 cm*1 cm). There is a rubber sheet of dimension (10 cm*10 cm) and current collectors in between two acrylic plates.

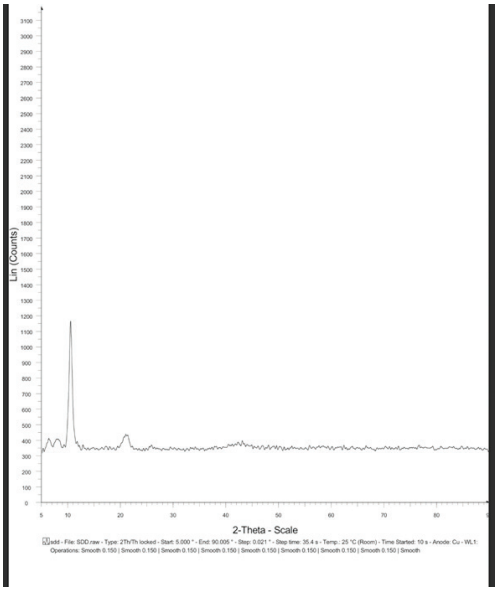


Figure 1: XRD of GO

Figure 2: Flow through capacitive deionization (CDI) set up

.Proposed Work in 2018-19

1. Study CDI of salt solution in flow through CDI set up at several voltages.
2. Study CDI of salt solution in flow between CDI set up at several voltages.

GAIKWAD GANESH ARJUN

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

Droplet microreactor designing and fabrication for Palladium nanoparticle synthesis is done. Palladium nanoparticle synthesis using fabricated droplet microreactor has been

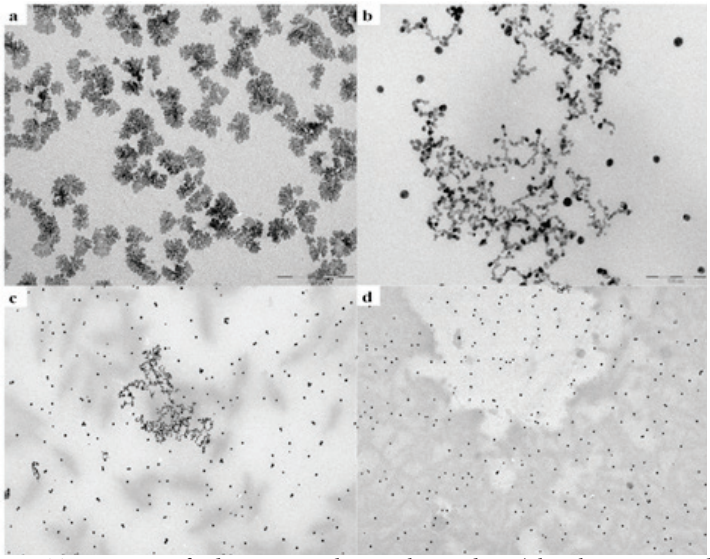


Fig1: TEM image of Pd nanoparticles synthesized in a) batch process and continuous process b) slug mode c) transition slug mode d) droplet mode

successfully carried out. Cellular uptake and toxicity studies for palladium nanoparticles have been conducted. Continuous synthesis of Pd nanoparticles was carried out in a droplet microreactor using sunflower oil as the continuous phase and a solution of sodium tetrachloropalladate (Na_2PdCl_4), L-Ascorbic acid sodium salt ($C_6H_7NaO_6$) and trimethyl chitosan (TMC) as the aqueous phase. The synthesis was carried in droplet, transition slug and slug flow for Na2PdCl4: ascorbic acid ratio of 1:2 and 2:5.

TEM morphology analysis (Fig1) shows that droplet synthesis gives uniform and spherical palladium nanoparticles compared to other modes. It can be inferred from study that TMC capped palladium nanoparticles is governed by self-assembly of TMC on pd nanoparticles during growth of nanoparticle.

Radiolabeling of functionalized chitosan oligosaccharide-DOTA nanoparticles was carried out. The radiolabeling yield was analyzed by paper chromatography technique. 0.05 M sodium citate solution was taken as the eluting agent. The radiolabeled nanoparticles remained at the point of spotting (R_f = 0-0.1) while free activity (177Lu3+) migrated to the solvent front (R_f = 0.8-1.0). The radiolabeling yield from the paper chromatogram was estimated to be ~ 65 %. However, the radiolabeled agent was unstable in PBS and the radiochemical purity decreased to ~ 5% on incubation in PBS medium for 10 minutes.

Work under progress:

Functionalization of Chitosan oligosaccharide nanoparticles with DOTA is under process to maximize radiolabeling. Also, the previously synthesized silver nanoparticles are to be conjugated with monoclonal antibody for targeted anticancer therapeutics. Further, the photo-thermal property of Pd nanoparticles for assessing their potential as theranostic agent is also in process for cancer treatment application.