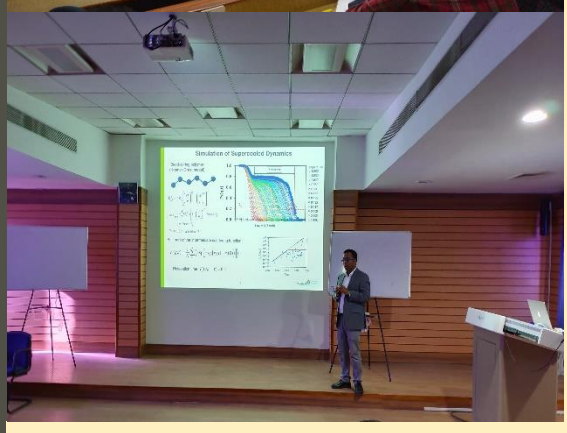

Newsletter

September - 2018

Indian Institute of Chemical Engineers

GUWAHATI REGIONAL CENTRE

Department of Chemical Engineering

IIT Guwahati

Battery Electric Vehicles in India: A Perspective

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The rising levels in pollution and energy demand due to increasing population, as well as from developments in science and technology, is clearly making sustainable energy as the paramount policy goal for our nation. However, most of our energy demand is currently met using fossil fuels and we depend largely on oil imports. Limited reserves of fossil fuels and the monopoly of their reserves in certain countries result in a volatile market. Moreover, the impact of fossil fuels on our health and environment is disastrous due to high amounts of particulate matter and oxides released during their usage. Road transportation accounts for a major share of our energy demand and CO_2 emissions [1]. Recent advancements in electric vehicles have been very positive and the potential of this emerging technology to replace IC engine vehicles has been discussed heavily in the literature as it can help us achieve a clean and sustainable environment at a low operational cost. However, being a nascent technology, as is the case with every new technology, it has various limitations that could hinder its success. Battery electric vehicles have been realized to be a reliable, cost-effective and clean option for day-to-day operations. Considering the reasonably high initial cost of the vehicle due to a higher cost of batteries and low demand for electric vehicles, the Government of India and some state governments have launched various subsidy schemes. The Government of India has also taken up various initiatives to improve research in the area of electric vehicles [1].

When India aims to produce and sell only electric vehicles by 2030, the major question to ask is whether it is possible to meet all our road transportation needs using electric vehicles or not. There are a lot of articles available that discuss the pros and cons of electric vehicles. As discussed above, they identify sustainability and low-cost operation as the most beneficial aspects of EVs. Most of these articles focus on lack of charging points due to a lower range of EVs, and longer charging times as the major demerits. Even if we built charging points in every possible parking location and reduce the charging times considerably, will it be possible to use EVs for all the transportation needs (private/public, long/short drives)?

Being working in the area of Li-ion batteries, I noticed that most of them failed to mention battery safety issues due to overheating or other reasons. I feel that safe operation of batteries is one of the major challenges that needs to be addressed if we would like this electric vehicle technology to replace traditional IC engine vehicles. I am doing my postdoctoral research at Columbia University (New York) and last month, they introduced electric buses for inter-campus shuttle services. One day during the travel, our driver suddenly stops the vehicle and says that the battery is overheated and we cannot move any further until it cools down. This happened early in the morning when the bus was on road for less than 2 hrs. It made me realize that we are still far away from using electric vehicles for public transport or taxis or for a long drive that requires continuous use of the battery. Even if we use a battery with high capacity and thus a high range, we may not be able to use that to its full potential due to this issue of overheating. Now, what happens if the battery gets overheated regularly? When we charge a battery at a higher current or voltage (to reduce charging time) or we use the battery continuously for longer hours, the battery gets overheated, just like our mobile phone batteries. A high temperature operation will increase the reaction rates giving rise to increased heat dissipation. This will further increase the battery temperature resulting in a positive feedback unless heat is removed at a faster rate than it is generated.

This positive feedback behavior can result in a thermal runaway. At around 800C, solid electrolyte interphase (SEI) layer will breakdown, exposing the carbon electrode to the electrolyte. This will result in an exothermic reaction between the electrode and the electrolyte, further increasing the temperature. If the temperature rises above 1000 ^{o}C, organic solvents might breakdown releasing flammable gases. Later, if the metal oxide electrode breaks down releasing O_2, flammable gases will catch fire and the battery will explode. These series of reactions in a battery are together referred to as thermal runaway [2,3]. Although the electric cars are equipped with controllers and cooling systems, possibility of a serious accident still exists. We all might have read that Federal Aviation Administration (FAA) grounded all Boeing 787s in 2013 after multiple incidents of battery fire. The root cause of these fires were later identified as short-circuit/thermal runaway in batteries. Like we did in our campus shuttle bus, we might have to wait for the battery to cool down every few hours to avoid this risk of overheating. But, it is not a convenient or practical solution for public transport buses or taxis. Later in the same year, Tesla Model S battery catches fire due to a puncture made by direct impact of a metallic object to one of the battery modules. These examples show the importance of heat management and other safety features in any application of batteries.

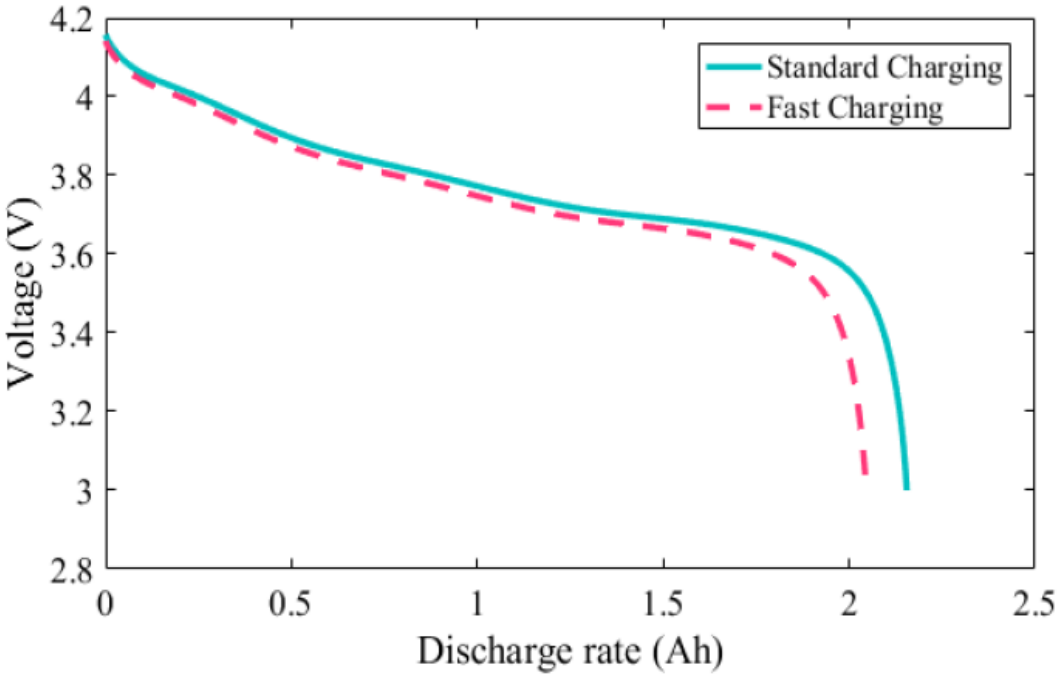

Figure 1: Comparison of battery charge-discharge profiles generated using first principles model after 150 cycles using fast charging (10 A) and standard charging scenarios (1 A) for a 1.67Ah battery. Model used incorporates 2 capacity fade mechanisms: SEI layer formation and Li plating. Capacity for fast charging is 5% lesser in comparison to standard charging case at 150th cycle [4]

In fact, overheating is one of the primary reasons for longer charging times which in turn is the reason for our need for a large number of charging stations. To lower charging time, we need to charge at a higher charging current which might result in overheating. In a study conducted during my PhD thesis, it was found that there is always a compromise between charging time and battery lifetime in deciding a charging rate as shown in Figure 1 [4]. Moreover, because of longer charging time and a large number of vehicles, if we need to accommodate charging requirements for many vehicles at a time, we need a large number of charging stations.

To summarize, although electric vehicle is an extremely significant technology, we are still far away from completely replacing IC engine vehicles with electric vehicles especially in case of public transports (buses/taxis) or long rides. We need to develop remarkably efficient heating management systems to ensure the safe operation of these EVs. Meanwhile what we all can do about sustainability is to rely more on public transport and less on private vehicles reducing pollution which reminds me of a famous quote: 'A developed country is not a place where the poor have cars; it's where the rich use public transportation'.

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Computational design of catalyst using ab-initio microkinetic modeling

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Heterogeneous catalysis shapes the establishment of the chemical industry. Catalysis is connected to numerous fundamental processes applied to the synthesis of essential substances and commodities we use in our normal lives. Heterogeneous catalysis is utilized to deliver an extensive variety of products from fuels, petrochemicals, fertilizers, plastics, pharmaceuticals etc. Heterogeneous catalyst also employed to clean our environment, such as cleaning the exhaust from automobiles, thermal power plants, industry waste and sewage, bio-waste etc.

As the heterogeneous catalysis occurs close to the active site and the electronic structure of the active site, it is conceivable to demonstrate it in an atomic scale with just few atoms representing the active site. With the advances in the modern electronic structure theory we now are able to compute the binding energies of the intermediates and activation barrier of any elementary reaction step with sufficiently high precision, so we can effectively model the complex catalytic process based on simple atomic scale ab-initio DFT calculation.

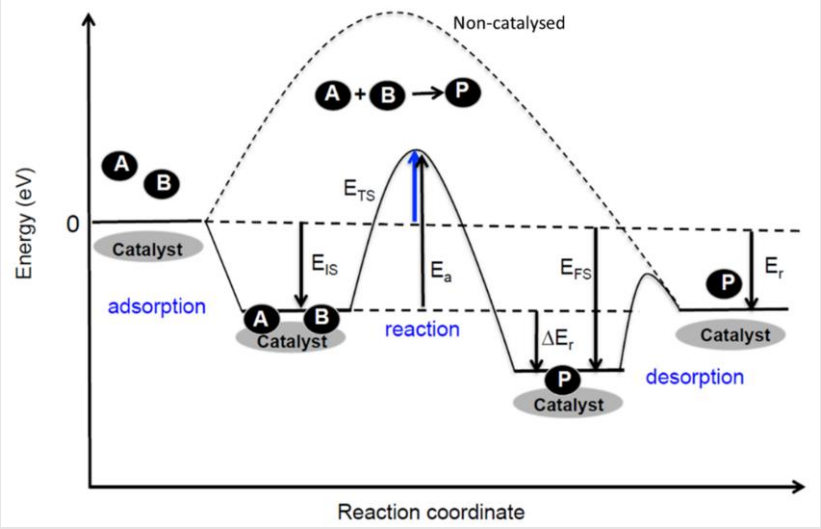

Figure 1: Schematic energy diagram for a chemical reaction of reactant A and B reacting on a catalyst surface to give product P. The general notations used here are, initial state energy (EIS), final state energy (EFS), transition state energy (ETS), activation barrier (Ea), reaction energy of elementary step (ΔEr) and overall reaction energy of the process (Er). Adapted from reference [1].

Heterogeneous catalysis in general works in a closed four-step process, first, the molecules of reactants get adsorbed at the catalyst surface or the active site, then the catalyst facilitates the dissociation of bonds between the reactant molecules, next it helps the dissociated species to react between themselves and make new bonds to form product molecules and finally the product molecules desorb from the surface.

Microkinetic modeling (MKM) is used to obtain the steady state kinetics, given that we provide the necessary input parameters like reaction conditions, gas-phase energies, adsorption energies and transition state energies, etc. MKM do not assume any elementary steps as the rate determining step. Catalytic processes usually consists of a number of elementary steps.

The adsorption energies of the intermediates and the transition state energies of the elementary steps are scaled against binding energies of most relevant intermediates, usually carbon, oxygen or nitrogen. The differential equations for each elementary steps is constructed based on the surface coverages of the species, forward and backward rate constants and concentration of the gas-phase species. For a given simulation we need to assume some realistic initial reaction condition and initial coverage, and then solve the coupled differential equations self-consistently until a steady state solution is obtained. More details on MKM can be found in CatMAP website https://github.com/SUNCAT-Center/catmap

Here I have presented three examples of successful implementation of ab-initio MKM to screening metallic and bimetallic alloy catalyst for industrially important processes.

Steam reforming of methane:

In the first example, I will discuss, steam reforming of methane, which is a very important reaction in chemical industry for hydrogen and syngas production. Hydrogen is one of the valuable chemical and widely used for making ammonia in fertilizer plants, for processing and upgrading petroleum crude, etc. Hydrogen also used as reducing agent in both organic and inorganic reactions. Syngas ($CO+H_2$) can be converted to fuel or alcohol using chemical synthesis. Though the process is already well established and few proven catalyst are in commercial production, there is always need of active, stable, and low-cost novel steam reforming catalysts.

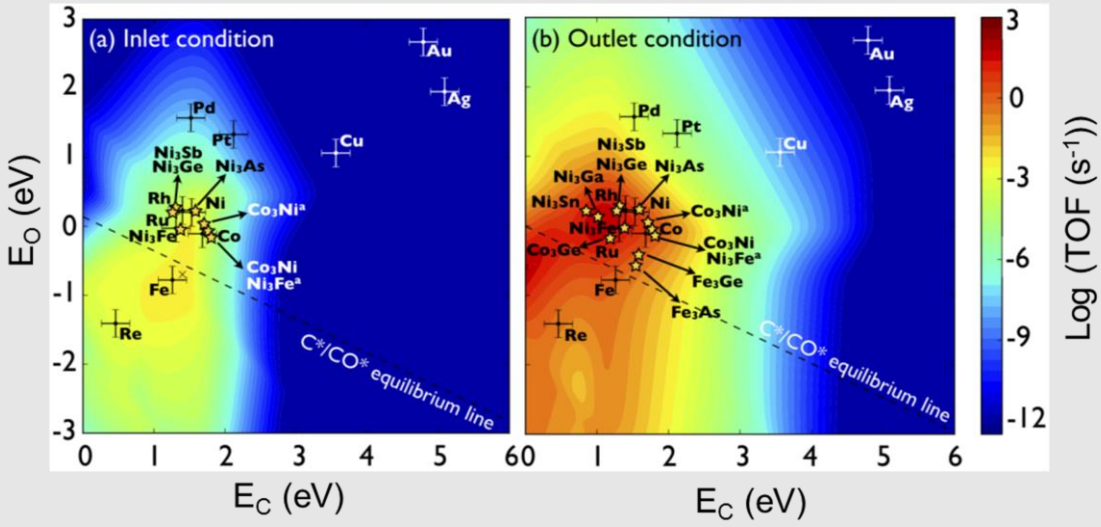

Figure 2: Calculated turnover frequencies (TOFs) for CO production during methane steam reforming under industrial (a) inlet conditions: T = 638 K, P= 14.3 bar, with a gas composition of 14.5% CH_4, 83.1% H_2O, 0.1% CO, 0.4% N_2, and 1.9% H_2 (corresponding to 0.3% approach to equilibrium); and (b) outlet conditions: T = 1066 K, P= 12.2 bar, with a gas composition of 2.4% CH_4, 65.8% H_2O, 6.5% CO, 0.3% N_2, and 25% H_2 (corresponding to 50% approach to equilibrium); as a function of C and O binding energies. Adapted from reference [2].

In this work, we used the descriptor-based microkinetic model to predict reaction rates in terms of the adsorption energies of carbon and oxygen. Using this model, we screened a large number of transition metal alloys based on their predicted rates and stabilities for CH_4 steam reforming. Of all screened alloys, Ni_3Fe, Co_3Ni, Ni_3Sn are known candidates for steam reforming reactions and have industrial application. Co-Ni and Co-Ge are reactive at both the inlet and outlet reactor condition, hence are the best candidates for CH4 steam reforming [2].

Hydrodeoxygenation of ethanol:

Due to the depleting fossil fuel reserve, ever increasing CO_2 levels causing environmental concern, conversion of biomass to fuel and chemical have got lot of attention worldwide in recent years, Platform molecules obtained from biomass are often found enriched with oxygen and require a suitable deoxygenation process for their conversion into high value chemicals and fuels.

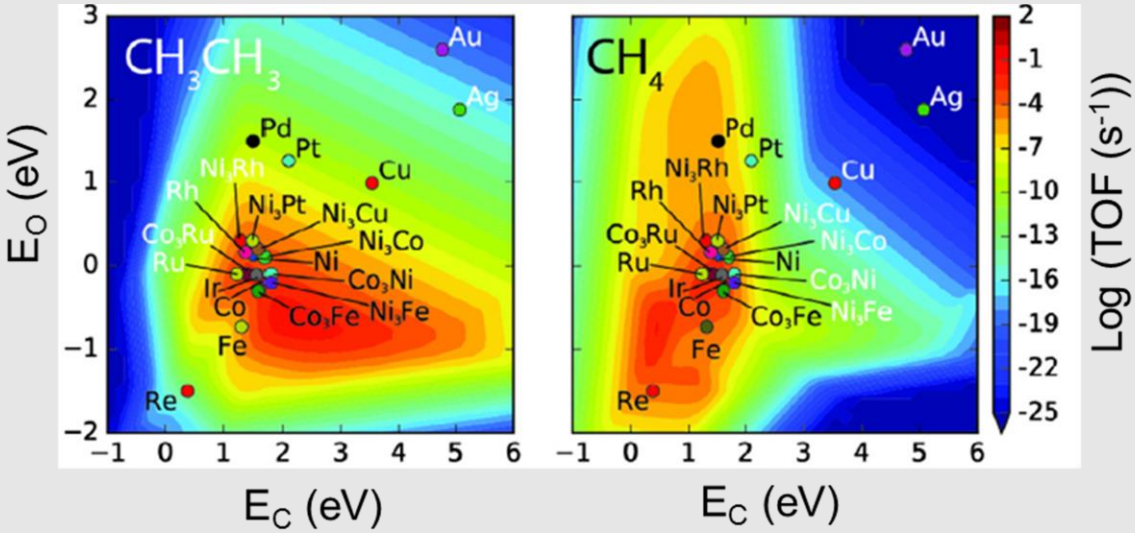

Figure 3: Calculated TOFs over bimetallic alloy catalysts for ethane and methane at reactor outlet temperature 523 K as a function of C and O binding energies during the HDO of ethanol. Pressure = 2 bar (50% CH_3CH_2OH and 50% H_2. Adapted from reference [3].

In the second example, ethanol was used as model compound to understand the catalytic activity and selectivity trends observed for the HDO reactions of biomass-derived platform molecules on supported metal catalysts, using carbon and oxygen binding energies as the descriptors. Ethanol conversion to ethane at 523 K over transition metal catalysts follows the order;

Co > Ru > Ir > Rh > Ni > Fe > Pt > Pd > Cu > Re > Ag > Au.

Significant conversion towards the HDO product ethane was observed. On applying the screening method on bimetallic alloys, Co_3Ni, Co_3Fe and Ni_3Fe, were found to show the high turnover of ethane (10^{-3} s^{-1}) while maintaining high HDO selectivity [3].

Oxidation of ammonia:

In recent years the selective oxidation of NH_3 has catch the interest both in the scientific community and industry for its potential applications in cleaning of NH_3 from air and developing better ammonia slip catalyst (ASC) for exhaust gas. Emission of NH_3 causes acidification of the environment in indirect ways. The acidification caused by NH_3 has already caused severe damage to the ecosystem in many countries like the Netherlands.

For this catalytic NH_3 oxidation study, we have used a 'dual facet' model as our catalysis surface. The 'dual facet' model surface is a combination of {111} terrace and {211} stepped surface. The adsorbates can adsorb on both the {111} and {211} and they are allowed to diffuse from one surface to another [1]. The catalytic trend for ammonia oxidation over transition metals obtained as,

Pd > Pt > Ag > Ru _ Au > Ni > Cu > Co > Fe > Re.

Pd and Pt have the highest NH_3 oxidation rate, indicating the common use of Pt in ammonia slip catalyst (ASC). Transition metals Ag. Rh, Cu, Ru and Ni shows moderate activity. Co, Fe and Re shows very little

activity, as the surface is poisoned by adsorbed oxygen.

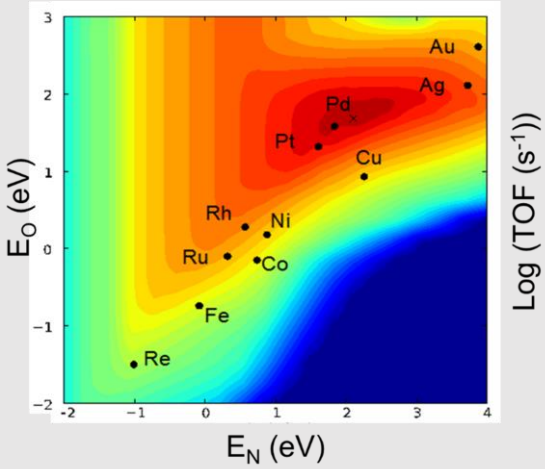

Figure 4: Catalytic rate of NH_3 oxidation (N_2 formation rate) on a ({111} + {211}) dual facet model surface is plotted versus the nitrogen and oxygen binding energies, EN and EO. The reaction condition is: T = 400 C, P= 1 bar, with a gas composition of 1980 ppm NH_3, 1985 ppm O_2, 10 ppm N_2, 30 ppm H_2O, 0.1 ppm H_2 (corresponding to 1% conversion from initial gas composition of: 2000 ppm NH_3, 2000 ppm O_2). Adapted from reference [1].

In future we aim to screen large number of metal alloy catalysts using the above established “in silico” catalyst screening approach.

Few other examples of successful implementation of MKM from our group at IIT Delhi are listed in the reference below [4,5].

In summary, with DFT calculated adsorption energies and activation barriers we can formulate an ab-initio microkinetic model to calculate intrinsic catalytic activity of an active site. Three distinct examples are presented here to emphasise on how we have successfully applied the MKM technique on catalytic reactions covering from high temperature, high pressure reforming reactions to low or moderate temperature biomass hydrodeoxygenation, expanding all the way to environmental catalysis like ammonia removal. This scaling based microkinetic model frame the base of the "in-silico" approach for the pursuit of new catalyst material of both industrial and environmental importance.

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Modified Hand Pump: An Emerging Cavitating Technology for Water Disinfection

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Water borne diseases is major concern in India. Large population of India is affected due to non-availability of sustainable technology for water disinfection for the people residing rural part of India. Conventional methods for water disinfection such as coagulation, filtration through porous media medium are not sufficient to address the emerging contaminants present in water [1]. Reverse osmosis – ultraviolet technologies is not affordable for large masses of people. Technologies based on cavitation phenomena has a potential to address the issues of water disinfection. Cavitation is phenomena of generation, growth and collapse of million cavities in liquid medium. At collapsing stage, it creates higher magnitude of temperature and pressure condition. These conditions are useful for microbial disinfection, removal of TDS and other contaminants present in water [2-4].

Overview of Water disinfection from Indian Context

India is second largest populated country and shares 17.5% of world population and holds 4% of fresh water. It is declining rapidly with human invasion through discharge of domestic and industrial wastewater in fresh water flowing in rivers. Hence, accesses to fresh water to 1.2 billion pollution is a difficult challenge [2]. Another concern is depletion of ground water sources scenario. Central pollution control board classified domestic use of water in two classes A and B. Class A is refereed as drinking water and B for bathing and other domestic use. Criteria for class A water is define based on following parameters [1]:

- Total coliform organism (MPN): less than 50
- pH range: 6.5 to 8.5
- Dissolved oxygen: more 6 mg/L
- Biochemical oxygen demand: 2 mg/L or less

Water disinfection using conventional methodology of filtration followed by chlorine dosing is limited to urban population and running effectively some of metropolitan cities. With unplanned grooming of urbanization, municipal corporations are not able to provide disinfected water to all parts of urban cities. It is reported nearly 60% of urban population residing in India is getting disinfected water and rest urban population depends on ground water source. Almost there is no disinfection facilities for rural India [3]. Most of rural India is depending on the Handpumps, Wells, etc. They are drinking water without any prior treatment and expose many diseases. Water in rural India is highly contaminated with microbial and heavy minerals. RO-UV system for water treatment is not effective for all. Hence, there is urgent need to address this issue using cavitational based technologies.

Indian researchers from Institute of Chemical Technology, Mumbai, Dr. Gogate, Prof. Pandit and from Indian Institute of Technology Guwahati, Prof. Moholkar, did the pioneer work in the field of cavitating technology. Their groups have explored cavitation for various chemical processing applications. Gogate (2007) written excellent review on the water disinfection using cavitation, he has presented economical analysis of water disinfection using acoustic and hydrodynamic cavitation [2]. According this analysis, acoustic cavitation is not cost-effective compare to conventional water disinfection technique whereas hydrodynamic cavitation has greater potential for water disinfection. Pandit and Kumar (2015) presented

excellent analysis of commercially available water disinfection products such as Tata Swach, Electrochemical arsenic remediation, Terafil, Ceramic filters, Tippu Taps, SODIS, Herbal based treatment and NEERI jar portable instant water filter [3]. They recommend that water disinfection technique should have community-based focus and there is need for development for community viable water disinfection techniques.

Hand Pump

In mid of 1960, Indian government had taken interest in providing adequate and safe water supply, especially in the large of villages. A miracle combination of borehole/hand pump as a source of drinking water to a large number of no-source situation in country. The hand pump is essentially a positive displacement pump, using negative pressure to lift water from bore well to surface level [3-6]. With higher dependency on ground water and industrialization quality of water delivered from hand pump is depleting. It has reported that hydrodynamic cavitation as energy efficient and economical method for treating bore well water. Hydrodynamic cavitation phenomena can be created at suction valve in hand pump and cavity generated by collapsing pressure of several orders bars. These pressures are sufficient for rupturing microbial/biological constitutes present in water. Suction valves in hand pump can be effectively used for possible disinfection of water while pumping water through system or reduce the microbial disinfection at the source [5-7]. Various suction valve design such as orifice plates, venturi, vortex diode, swirling jet etc may be used. Selection of suction valve is depending on reduction of microbial activity in water with lesser pressure loss and minimum hand pump lift [5-6]. The important design parameters contribute to modified design of hand pump are available flow area as function of lift, and head diameter of the check valve.

Start-up in Modified Hand Pump [8]

Taraltec solution is one of the start-up company working in the field of design of hand pump. They claimed that 99% microbial free disinfected water with cavitating reactor for hand-pump. Their product has been selected as one of the four start-ups by government think tank Niti Aayog to represent the country at an India-Israel tech innovation exhibition on water, health and agriculture. This product is design based on principal of hydrodynamic cavitation and fitted as additional part in the conventional hand pump. They are selling this product at the cost of Rs. 6000/- and time required for installation is 15 minutes.

Modified hand pumps based on hydrodynamic cavitation is one of the promising options, to address the challenges in water disinfection for large community. Ground water quality in all parts of India is not same, some part is highly contaminated with minerals like arsenic, fluoride and microbial contamination. One common design of hydrodynamic cavitation is not sufficient to address water disinfection issues in India. Hence, there is need for more research groups and start-ups.

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Optimization of Production Planning Industries using Computational Intelligence Techniques

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Optimization is one of the most important quantitative tool, which plays a crucial role in industrial decision-making. A variety of problems in the production planning, process flowsheeting, designing, and analysing of chemical plants can be efficiently solved by using optimization techniques. The benefits of using optimization techniques in chemical processes and plants can be observed in numerous ways such as determining the best site for plant location, allocating resources or services among several processes, evaluating the plant data to construct a model of a process etc. [1].

Production planning industries have complex networks of different processes and resources that are available to convert feedstocks such as crude oil into primary products such as benzene, toluene, xylene etc. However, these primary products can be used as a raw material for the production of other intermediate and final products. The flexibility in the production of a product and the availability of many process technologies offer the sense of switching between production methods and raw materials utilized. Due to the increasing cost of energy, raw material availability and other factors, which affects the production, the major objective is to improve the efficiency of existing plants and maximize the utilization of available resources to achieve the maximum revenue. The aim of a production plan is to generate maximum revenue with the production of valuable products along with the optimally utilizing the available resources and the satisfaction of the other constraints associated with the production plan such as satisfying the market demand, unique process constraint etc. Production planning plays an essential role in production management framework and is a key region of global business operations management. The goal of the optimization techniques in the production planning is to make the decision about what products must be produced, the amount of the products needed to be produced, and the processes to be employed to produce the selected products. To determine the best configuration among the available route to produce particular products is the primary aim of a production-planning model. Petroleum refineries and the basic petrochemical industries are the most energy-intensive processes in the chemical process industry. More than 660 refineries in 116 countries are currently in operation and producing more than 85 million barrels of refined products per day [2]. In the present scenario, the petroleum and the chemical industries fall in the category of pollution incentive industries and renewable greener technologies hold the supremacy over these industries with the use of renewable resources for the production of daily life consumable products such as biodiesel production fuel made from vegetable oil [3]. Therefore, with an increase in competition from renewable sources, production-planning industries has become mandatory to remain competitive and profitable.

Production planning is a combinatorial optimization problem that had been successfully solved by using the mathematical programming. In mathematical programming, the production-planning model needs to be formulated in terms of conventional optimization form in which the constraints associated with the production-planning model need to be postulated in terms of equalities and inequalities. The successful implementation of mathematical programming in production planning problems can be found in the literature such as a generalized network flow MILP model using a sequence-dependent setup approach to model and solve capital investment planning problems, nonlinearities are approximated to linearized operations [4]. MILP model for maximising profit with the satisfaction of resource and other

and other constraints, which aids in guiding petrochemical industries in Saudi Arabia [5].

A real-life engineering based optimization problem is difficult to formulate in the generalized form of mathematical programming. However, the formulation of complex constraints in the form of conventional equalities and inequalities is a bit challenging one especially for nonlinear functions. CI techniques provide the flexibility to formulate the complex constraints such as nonlinear functions, conditional constraints and do not enforce the constraint to formulate in conventional equality and inequality form. CI techniques are also capable of solving the complex back box optimization problems [6]. In CI techniques, for every iteration, the set of solutions (decision variables), whose fitness is to be determined using the problem statement, the fitness value of the decision variable is to be returned to the CI techniques, which will utilize the information to explore for better solutions. The relation between CI techniques and the problem statement can be observed from Fig 1. Some instances of artificial intelligence based optimization techniques in real life engineering production planning problem can be found in the literature such as the development of the petroleum exergy production and consumption relations for better utilization of exergy and predicts the future estimations by using simulated annealing approach [7], multi-unit production planning problem based on continuous variables [8]..

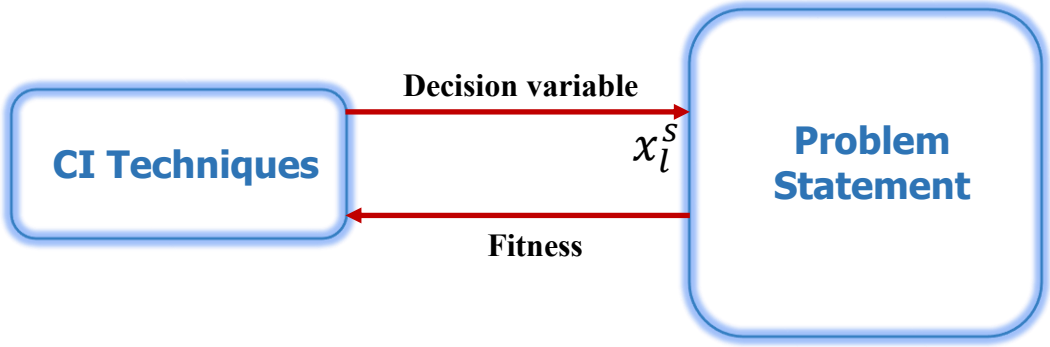

Figure .1. Information flow between CI technique and the combinatorial production-planning problem

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Guwahati Regional Centre Activities

Seminar Series on *Physics of draining in the meso-scale: Experimental and theoretical analysis*

Prof. Gargi Das, Department of Chemical Engineering, IIT Kharagpur delivered this talk on April 3, 2018.

The phenomenon of draining, although ubiquitous in nature, has received scant attention especially in the meso-scale. We observe that closed top tubes drain by the inception of an axisymmetric 'Taylor finger' while a minute pierce of the top closure results in an altogether different physics with air entry from the top pushing the liquid out. A coupled mechanism combining full bore and film draining is observed for "too small" a top pierce at "high enough" Eotvos number. Top pierce initiates draining in dimensions which would not drain otherwise and finger entry hastens the process of draining. The myriad of phenomena thus exhibited is depicted as phase diagrams in vertical and tilted conduits. A mechanistic model has been proposed to predict draining and the onset of finger entry in vertical tubes.

Seminar Series on *comparative analysis of water purification technologies*

Dr. Jaideep Chatterjee, Principal Scientist, Unilever and Adjunct Faculty of Department of Chemical Engineering, IIT Guwahati delivered this talk on April 27, 2018.

A brief review of the evolution of potable water purification and waste-water purification technologies is presented. The current most popular technologies for potable water purification are presented. The theoretical basis of the most popular current technology is discussed in some details. The limitations of reverse osmosis technology are also discussed. The variability of the specific energy consumption with recovery is also discussed. Some simple techniques for improving recovery while optimizing specific energy consumption are also discussed. The importance of scale prevention is highlighted. Current technology status for practical in-home water softening is also discussed.

Seminar Series on *Micro-physiological models that mimic mucosal barrier complexity of the human intestine*

Mr. Abhinav Sharma, Research Scholar, University of Massachusetts Amherst delivered this talk on April 27, 2018.

The mucosal barrier in the intestine is vital to maintain selective absorption of nutrients while protecting internal tissues and maintaining symbiotic relationship with luminal microbiota. This bio-barrier essentially consists of a cellular epithelial barrier and an acellular mucosal barrier. While formation of a mucus barrier is dependent on mucin secreting goblet cells, secreted mucin biopolymers regulate barrier function via in situ biochemical and biophysical interaction with luminal content that continually evolves during digestion and absorption.

Increasing evidence suggests that a mucus barrier is indispensable to maintain dynamic homeostasis of the gastrointestinal tract. However, the importance of mucus barrier has been largely underrated for in vitro mucosal tissue modeling. The major gap is the lack of experimental material (i.e. functional mucins) and platforms to integrate a relevant thickness of mucus layer with an epithelium under physiologically related conditions. In the presentation I shall discuss our progress on developing human-relevant micro-physiological mucosal barrier models in static and dynamic

To overcome limited availability of functional mucus, we developed a simple and scalable protocol for natural mucus extraction by directly solubilizing a relatively sterile inner mucus layer from porcine small intestines (PSI) that is readily accessible.

Seminar Series on *An introduction about IGCAR and nuclear energy*

Dr. N. Sivaraman, Indira Gandhi Centre for Atomic Research delivered this talk on July 2, 2018.

An introduction about IGCAR and nuclear energy will be highlighted. Overview of the Fuel Chemistry Division activities with respect to nuclear fuel reprocessing program will be discussed in the presentation. General information on the atoms to manhattan project and contributions of various nobel laureates to the nuclear energy program will be presented.

Seminar Series on *Tribo-Electrostatic and its Application in Fine Coal Preparation*

Dr. R. K. Swari, Scientist, Mineral Processing Department, CSIR IMMT, Bhubaneswar delivered this talk on July 2, 2018.

Coal is the major resource of energy for the power generation and steel production. The depleted coal grade is required to process for its efficient industrial application. Dry beneficiation has several advantages over a wet process. In recent years, much research effort is aimed at dry processing of fine coal particles using the tribo-electrostatic separator. This technique has great potential to treat Indian coal fines. This is a two-step process in which particles are tribo-charged and then separated in an electric field. During tribo-charging, the particles are charged by frictional contact with each other or with the surface of other material. The polarity and magnitude of charge acquired by the particle are based on their work function difference on contact. Several factors affect the efficiency of tribo-electrostatic separators such as particulate physical properties, environment relative humidity and operating variable of tribo-charger and separator. Indian coal belongs to drift origin and has difficult liberation characteristics. The coal particulates liberated at finer sizes. Also, the particle size is crucial to obtain higher differential charging during tribo-electrifications for their efficient separation. Tribo-charging and environment relative humidity also greatly influence the charge characteristics of mineral and maceral. The particle size, density, charge and free fall separator electrode plate position and the potential gradient between them decide the particle trajectory and their separation in the electric field. Therefore, detail investigations required to develop a tribo-electrostatic process for fine coal preparation.

Seminar Series on *Molecular Design of Polymeric Ionic Liquids*

Dr. Tarak Patra, Center for Nanoscale Materials, Argonne National Laboratory, USA delivered this talk on September 14, 2018.

Polymeric ionic liquids (PILs) are very promising materials to enable more environmentally stable high-density energy storage devices. Realization of PILs providing high environmental and mechanical stability while maximizing ion conductivity would be accelerated by an improved molecular level understanding of their structure and dynamics. Extensive evidence suggests that both mechanical properties and ion conductivity in anhydrous PILs are intimately related to the PILs' glass formation behavior. This represents a major challenge to the rational design of these materials, given that the basic nature of glass formation and its connection to molecular properties remains a substantial open question in materials science and engineering. Here, I describe coarse-grained and atomistic molecular dynamics simulations probing the relationship between PIL architecture and

interactions, glass formation behavior, and ion transport characteristics while establishing machine learning frameworks for rapid, computationally-driven design of new materials.

Other Events

The Department of Chemical Engineering, IIT Guwahati and the Indian Institute of Chemical Engineers - Guwahati Regional Centre organized a one day event "State-of-the-Art in Refinery Operations" in association with Guwahati Refinery on April 4, 2018. The event consisted of seven lectures (four lectures from experts of Guwahati Refinery and three lectures from experts of IIT Guwahati).

One day workshop on ANSYS

The Department of Chemical Engineering, IIT Guwahati and the Indian Institute of Chemical Engineers - Guwahati Regional Centre organized a one day ANSYS workshop on September 1, 2018. The workshop included a hands-on session from the resource persons from ANSYS.

One day workshop on Applied Optimization

The Department of Chemical Engineering, IIT Guwahati and the Indian Institute of Chemical Engineers - Guwahati Regional Centre organized a one day workshop on Applied Optimization on September 29, 2018. The workshop included a hands-on session on the optimization toolbox of MATLAB. In addition, algorithms which have been recently reported in literature (and not available in MATLAB) were discussed.

We invite articles for the upcoming newsletter. Please write to iiche.grc@iitg.ernet.in for further details. The articles are published as provided by the authors. The opinions expressed in the articles should not be considered as endorsed by Indian Institute of Chemical Engineers – Guwahati Regional Centre or Indian Institute of Technology Guwahati.

IIChE newsletter is available at http://www.iiche.org.in/pdfs/NLVol9.pdf


SUMMARY


Physics of draining in the meso-scale: Experimental and theoretical analysis
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